ASYMPTOTICS IN TIME, TEMPERATURE AND SIZE FOR OPTIMIZATION BY SIMULATED ANNEALING: THEORY, PRACTICE AND APPLICATIONS

AFOSR-88-0181

FINAL TECHNICAL REPORT

Principal Investigators

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I. Summary of Research Accomplishments

This project was concerned with simulated annealing, a Monte Carlo method for obtaining globally optimal or nearly globally optimal solutions to a variety of optimization problems.

We have achieved key results in two main areas:

i) characterizing the cooling rate necessary and sufficient for simulated annealing to hit the global minimum, and

ii) obtaining a novel upperbound for the time-constant of convergence of simulated annealing at a fixed temperature to its equilibrium distribution and studying the growth of this bound as the temperature approaches zero asymptotically.

Simulated annealing with a time varying temperature gives rise to a time inhomogeneous Markov chain. This Markov chain is difficult to analyze and study due to the time-inhomogeneity. We have been able to obtain a novel theory for analyzing such processes. We have introduced a notion of "recurrence order" associated with each state of a Markov chain. Essentially, this recurrence order characterizes the rate of convergence of the occupation probability for the state. Our central result consists of the discovery that these recurrence orders satisfy a "balance equation" across every cutset of the graph of the chain for the general class of such Markov chains. For the special case of simulated annealing with symmetric neighborhoods, they even satisfy a "detailed balance" for every pair of states.

These balance equations transform the analytical problem of determining the asymptotic behavior of simulated annealing into a purely algebraic problem of solving the balance equations. We have obtained graph theoretic algorithms for solving such balance equations in general, and for simulated annealing in particular have obtained explicit solutions.

From the explicit solutions to the balance equations we have been able to characterize, i.e., obtain the necessary as well as sufficient condition for, the cooling rate in order for simulated annealing to hit

the global minimum of the optimization problem with probability one.

The above results are detailed in [1-3] of the attached list of Publications.

The behavior of simulated annealing at a *fixed temperature* can be modeled by a *reversible time-homogeneous* Markov chain converging to an equilibrium distribution at that temperature. As the temperature goes to zero asymptotically, the equilibrium distributions themselves converge to the optimal distribution. In [4], we have obtained a novel upper bound for the second largest eigenvalue of a finite reversible time-homogeneous Markov chain as a function of three parameters, namely, the smallest transition probability, the underlying structure of the chain, and the skewness of the equilibrium distribution. This eigenvalue bound enables us to bound the time-constant of convergence of a reversible Markov chain to its equilibrium distribution. In particular, we can bound the time constant of convergence of a fixed-temperature simulated annealing algorithm solving a particular instance of an optimization problem. Moreover, we can study the growth of this bound as the temperature approaches zero or skewness becomes arbitrarily large; thereby, providing a fairly good understanding of the *temperature asymptotics* of the simulated annealing algorithm. We exhibit a class of Markov chains on which our bound, treated as a function of skewness alone, is asymptotically tighter than previously established bounds based on a certain parameter known as the *conductance* of the Markov chain. We also show that our bound is, in general, much easier to compute for simulated annealing chains.

More recently, we have achieved what we believe to be a significant breakthrough in understanding the *size-asymptotics* of a time-homogeneous simulated annealing chain solving a particular combinatorial optimization problem known as the Integer Knapsack problem. For this NP-Hard problem, we have been able to derive sufficient conditions under which the time-constant of convergence of a fixed-temperature simulated annealing chain is a polynomial in the size of the problem. Combining this with an in-depth study of cost distributions and density of states, we have shown that for certain versions of the Integer Knapsack problem, a fixed-temperature simulated annealing algorithm can find a

state with cost sufficiently close to the global minimum in polynomial time with overwhelming probability. The manuscript containing these results is still under preparation and will be made available as soon as it is ready for publication.

PUBLICATIONS

1. D. P. Connors and P. R. Kumar, "Simulated Annealing Type Markov Chains and their Order Balance Equations," *SIAM Journal on Control and Optimization*, vol. 27, no. 6, pp. 1440-1462, November 1989.

2. D. P. Connors and P. R. Kumar, "Simulated Annealing Type Markov Chains and their Order Balance Equations," *Proceedings of the Twenty-Seventh Conference on Decision and Control*, pp. 1496-1501, Austin, TX, December 7-9, 1988.

3. P. R. Kumar, "Simulated Annealing and Balance of Recurrence Orders," *Proceedings of the SPIE Symposium: High Speed Computing III, pp. 103-106, vol. 1058, Keith Bromley, Editor, Los Angeles, CA, January 17-18, 1989.*

4. M. P. Desai and V. B. Rao, "A New Eigenvalue Bound for Reversible Markov Chains with Application to the Temperature-Asymptotics of Simulated Annealing," (accepted and to appear in) *Proceedings of the 1990 International Symposium on Circuits and Systems*, New Orleans, LA, May 1990.

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Generalized simulated-annealing type Markov chains where the transition probabilities are proportional to powers of a vanishing small parameter are considered. An "order of recurrence," which quantifies the asymptotic behavior of the state occupation probability is associated with each state. These orders of recurrence satisfy a fundamental balance equation across every edge-cut in the graph of the Markov chain. Moreover, the Markov chain converges in a Cesaro-sense to the set of states having the largest recurrence orders. These results convert the analytic problem of determining the asymptotic properties of the time-inhomogeneous stochastic process into a purely algebraic problem of solving the balance equations to determine the recurrence orders.

Graph theoretic algorithms are provided to determine the solutions of the balance equations. By applying these results to the problem of optimization by simulated annealing, it is shown that the sum of the recurrence order and the cost is a constant for all states in a certain connected set, whenever a "weak-reversibility" condition is satisfied. This allows

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We consider generalized simulated-annealing type Markov chains where the transition probabilities are proportional to powers of a vanishing small parameter. One can associate with each state an "order of recurrence" which quantifies the asymptotic behavior of the state occupation probability. These orders of recurrence satisfy a fundamental balance equation across every edge-cut in the graph of the Markov chain. Moreover, the Markov chain converges in a Cesaro-sense to the set of states having the largest recurrence orders. We provide graph theoretic algorithms to determine the solutions of the balance equations. By applying these results to the problem of optimization by simulated annealing, we show that the sum of the recurrence order and the cost is a constant for all states in a certain connected set, whenever a "weak-reversibility" condition is satisfied.

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SIMULATED ANNEALING TYPE MARKOV CHAINS AND THEIR ORDER BALANCE EQUATIONS*

DANIEL P. CONNORS† AND P. R. KUMAR‡

Abstract. Generalized simulated-annealing type Markov chains where the transition probabilities are proportional to powers of a vanishing small parameter are considered. An "order of recurrence," which quantifies the asymptotic behavior of the state occupation probability, is associated with each state. These orders of recurrence satisfy a fundamental balance equation across every edge-cut in the graph of the Markov chain. Moreover, the Markov chain converges in a Cesaro-sense to the set of states having the largest recurrence orders. These results convert the analytic problem of determining the asymptotic properties of the time-inhomogeneous stochastic process into a purely algebraic problem of solving the balance equations to determine the recurrence orders.

Graph theoretic algorithms are provided to determine the solutions of the balance equations. By applying these results to the problem of optimization by simulated annealing, it is shown that the sum of the recurrence order and the cost is a constant for all states in a certain connected set, whenever a "weak-reversibility" condition is satisfied. This allows the necessary and sufficient condition for the optimization algorithm to hit the global minimum with probability one to be obtained.

Key words. simulated annealing, optimization, Markov chains

AMS(MOS) subject classifications. 60J10, 90C27

1. Introduction. We consider finite state Markov chains $\{x(t)\}$ with transition probabilities of the type

$$p_{ij}(t) = c_{ij}\varepsilon(t)^{V_{ij}},$$

where $\varepsilon(t)$ is a small parameter converging to zero. In a previous paper [7] we have shown that if we define "orders of recurrence" by (more precise definitions are given in § 2)

$$\beta_i := \sup\left\{c \geq 0: \sum_{t=0}^{\infty} \varepsilon(t)^c \pi_i(t) = +\infty\right\},$$

then

(i) These recurrence orders satisfy a balance equation, $\max_{i \in A, j \in A^c}(\beta_i - V_{ij}) = \max_{i \in A, j \in A^c}(\beta_j - V_{ji})$, for every subset A; and

(ii) The Markov process converges to the set of states with the largest orders of recurrence.

This provides a novel approach to analyzing the asymptotic behavior of such time-inhomogeneous Markov processes. Specifically, we use (i) to solve the balance equations, and then (ii) provides the limiting behavior. Moreover, the orders of recurrence also provide information about the rates of convergence of the state occupation probabilities. This approach via recurrence orders therefore converts the analytic problem of determining the asymptotic behavior of the time-inhomogeneous process into a purely algebraic problem of solving the balance equations.

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A significant motivation for studying such Markov chains lies in the fact that in the method of optimization by simulated annealing, if $\{W_i\}$ is the cost function whose minimum is sought, then we obtain a Markov chain with

$$p_{ij}(t) = c_{ij}\varepsilon(t)^{\max(0, W_j - W_i)}.$$

Thus simulated annealing is a special case where the powers V_{ij} satisfy

$$V_{ij} := \max(0, W_j - W_i),$$

for some $\{W_i\}$.

To pursue the above approach to analyzing such time-inhomogeneous Markov chains, it is necessary to be able to solve the balance equations. However, there can be nonunique solutions to the balance equations. We present graph-theoretic circulation based algorithms to obtain *a* solution, as well as *all* solutions, to the balance equations. We show by an example the interesting phenomenon that such nonuniqueness can arise when the asymptotic properties of the Markov process, and the recurrence orders, depend not just on the *exponents* V_{ij}, but also on the *proportionality constants* c_{ij}.

By applying these results to the Markov chain arising from the method of optimization by simulated annealing when the "weak reversibility" condition of Hajek [1] holds, we show that the sum of the recurrence order and the cost is a constant on sets connected by recurrent arcs. This allows us to obtain the necessary and sufficient condition for the optimization algorithm to hit the global minimum with probability one. Our necessity result is a stronger sample path result than is found in [1] or [2].

Background. Tsitsiklis [2] has also investigated Markov chains with transition probabilities proportional to powers of a small time-varying parameter. His analysis was based on observing that due to the slow variation of $\{\varepsilon(t)\}$, we can employ bounds on the state occupation probabilities for *stationary* Markov chains, where $\varepsilon(t)$ is held constant, to obtain bounds for the time-inhomogeneous case. His approach is quite different from ours.

Based on an analogy to the physical process of annealing, the sequence $\varepsilon(t)$ is called the "cooling schedule," and just as in the physical analogy it plays a key role in determining asymptotic behavior. It has been shown by Geman and Geman [3], Mitra, Romeo, and Sangiovanni-Vincentelli [4], and Gidas [5], that simulated annealing converges in probability to a minimum of the optimization problem provided $\sum_{t=0}^{\infty} \varepsilon(t)^p = +\infty$ for large enough p. Hajek [1] has determined the necessary and sufficient conditions on the value of p for the algorithm to converge *in probability* to the minimum when a "weak reversibility" assumption is satisfied.

2. Orders of recurrence and balance equations. Consider a Markov chain over a finite state space X whose transition probabilities are proportional to *powers* of a vanishing time varying parameter $\varepsilon(t)$; that is, the transition probabilities $p_{ij}(t) := \Pr(x(t+1) = j \mid x(t) = i)$ are given by

$$(1) \qquad p_{ij}(t) = c_{ij}\varepsilon(t)^{V_{ij}} \quad \text{for all } i, j \in X,\ i \neq j, \text{ and } t \in \mathcal{T}^+, \text{ and } p_{ii}(t) = 1 - \sum_{j \neq i} p_{ij}(t)$$

where

$$(2) \qquad 0 \leqq V_{ij} \leqq +\infty \quad \text{for all } i, j \in X,\ i \neq j,$$

$$(3) \qquad c_{ij} \geqq 0 \quad \text{for all } i, j \in X,\ i \neq j, \text{ and } \sum_{j} c_{ij} = 1 \text{ for all } i.$$

Regarding the small parameter $\{\varepsilon(t)\}$, we will assume that,

$$0<\varepsilon(t)<1 \quad \text{for all } t\in\mathcal{Z}^+, \tag{4}$$

$$\exists M<\infty \text{ such that } \varepsilon(t)\leqq M\varepsilon(s) \text{ whenever } t\geqq s, \text{ and} \tag{5}$$

$$\sum_{t=1}^{\infty}\varepsilon(t)^p<\infty \quad \text{for some } p\in[1,+\infty). \tag{6}$$

In what follows we will assume that in (1)-(3) we have

$$c_{ij}=0\Leftrightarrow V_{ij}=+\infty,$$

which is clearly without any loss of generality. We shall denote by N_i the set of all states j with $c_{ij}>0$. Finally, we will assume that the Markov chain is "connected;" i.e., for every $i,j\in X$, there exists a path $i=i_0,\cdots,i_p=j$, with $i_l\in N_{i_{l-1}}$ for $1\leqq l\leqq p$.

Let $\pi_i(t):=\Pr(x(t)=i)$ be the probability distribution of $x(t)$, and let $\pi_{ij}(t):=\Pr(x(t)=i, x(t+1)=j)$ be the probability of a *transition* from state i to j at time t.

The following example motivates the notion of "orders of recurrence" introduced in [7].

Example 1. Suppose, for a certain Markov chain (with more than two states!), we have

$$\pi_1(t)=1/t^{1/3},\quad \pi_2(t)=1/t^{2/3},\quad \varepsilon(t)=1/t^{1/3}.$$

Then note that $\sum_{t=0}^{\infty}\varepsilon(t)^c\pi_1(t)$ is *finite* if $c>\beta_1:=2$ and $+\infty$ if $c\leqq\beta_1$. Similarly, $\sum_{t=0}^{\infty}\varepsilon(t)^c\pi_2(t)$ is *finite* if $c>\beta_2:=1$ and $+\infty$ if $c\leqq\beta_2$. Now $\pi_1(t)$ converges to zero more slowly than $\pi_2(t)$ and it is easy to see that this information is also captured by the demarcation points β_1 and β_2, which thus provide a measure by which to rank the rates at which $\pi_1(t)$ and $\pi_2(t)$ converge to zero.

Motivated by this we define the *recurrence orders* for the states and transitions of the Markov process, as follows.

DEFINITION 1. The order of recurrence of a state $i\in X$, denoted β_i, is

$$\beta_i:=\begin{cases}-\infty & \text{if } \sum_{t=0}^{\infty}\pi_i(t)<+\infty,\\ p & \text{if } p=\sup\left\{c\geqq 0:\sum_{t=0}^{\infty}\varepsilon(t)^c\pi_i(t)=+\infty\right\} \text{ and } \sum_{t=0}^{\infty}\varepsilon(t)^p\pi_i(t)<+\infty,\\ p & \text{if } p=\max\left\{c\geqq 0:\sum_{t=0}^{\infty}\varepsilon(t)^c\pi_i(t)=+\infty\right\}.\end{cases}$$

We say a state i is *transient* if $\beta_i=-\infty$; otherwise we say the state is *recurrent*.

In a similar manner we define the *order of recurrence of the transition from i to j*.

DEFINITION 2. The order of recurrence of the transition from state i to j, denoted β_{ij}, is

$$\beta_{ij}:=\begin{cases}-\infty & \text{if } \sum_{t=0}^{\infty}\pi_{ij}(t)<+\infty,\\ p & \text{if } p=\sup\left\{c\geqq 0:\sum_{t=0}^{\infty}\varepsilon(t)^c\pi_{ij}(t)=+\infty\right\} \text{ and } \sum_{t=0}^{\infty}\varepsilon(t)^p\pi_{ij}(t)<+\infty,\\ p & \text{if } p=\max\left\{c\geqq 0:\sum_{t=0}^{\infty}\varepsilon(t)^c\pi_{ij}(t)=+\infty\right\}.\end{cases}$$

Again, we say the transition from i to j is *transient* if $\beta_{ij}=-\infty$; otherwise we say the transition is *recurrent*.

It is also convenient to define ρ, the *order of cooling* of $\{\varepsilon(t)\}$, as follows.

DEFINITION 3. The order of the cooling schedule $\{\varepsilon(t)\}$, denoted ρ, is defined as

$$\rho := \begin{cases} -\infty & \text{if } \sum_{t=0}^{\infty} \varepsilon(t) < +\infty, \\ p & \text{if } p = \sup\left\{c \geq 0: \sum_{t=0}^{\infty} \varepsilon(t)^c = +\infty\right\} \text{ and } \sum_{t=0}^{\infty} \varepsilon(t)^p < +\infty, \\ p & \text{if } p = \max\left\{c \geq 0: \sum_{t=0}^{\infty} \varepsilon(t)^c = +\infty\right\}. \end{cases}$$

The relationship between β_i, β_{ij}, and ρ is given in the following lemma. It will be convenient in the sequel to define the operation "$\ominus$" as follows:

$$a \ominus b := \begin{cases} -\infty & \text{if } a < b, \\ a - b, & \text{if } a \geq b. \end{cases}$$

LEMMA 1. *β_{ij} and β_i are related by*

$$\beta_{ij} = \beta_i \ominus V_{ij} \quad \text{for all } i, j \in X, \tag{7}$$

while ρ and β_i are related by

$$\max_{i \in X} \beta_i = \rho. \tag{8}$$

Proof. If $j \notin N_i$, then it immediately follows that $\beta_{ij} = -\infty$. If $j \in N_i$, then application of the Chapman-Kolmogorov equation

$$\begin{aligned} \pi_{ij}(t) &= \pi_i(t) p_{ij}(t) \\ &= c_{ij} \varepsilon(t)^{V_{ij}} \pi_i(t), \end{aligned}$$

gives the first assertion. Similarly, since

$$\sum_{t=0}^{\infty} \varepsilon(t)^p = \sum_{i \in X} \sum_{t=0}^{\infty} \varepsilon(t)^p \pi_i(t),$$

the second assertion also follows. □

Knowledge of the β_i's provides useful information about the asymptotic properties of $\{x(t)\}$. The following theorem shows that the time-inhomogeneous Markov chain converges in a *Cesaro sense* to the set of states having the largest orders of recurrence.

THEOREM 1. *Let $\mathcal{M}$ be the set of states with the largest orders of recurrence:*

$$\mathcal{M} := \{i \in X: \beta_i = \rho\}.$$

Then

$$\limsup_{N \to \infty} \frac{1}{N} \sum_{t=1}^{N} \Pr(x(t) \in \mathcal{M}) = 1. \tag{9}$$

Proof. Let us first consider the set $\bar{\mathcal{M}}$ defined by

$$\bar{\mathcal{M}} := \begin{cases} \mathcal{M} & \text{if } \rho = 0, -\infty \text{ or } p \text{ for some } p \in \mathcal{R},\ p > 0, \\ \mathcal{M} \cup \{i \in X: \beta_i = p\} & \text{if } \rho = p \text{ for some } p \in \mathcal{R},\ p > 0. \end{cases}$$

Note that if $\rho = p$, then $\bar{\mathcal{M}}$ may be slightly larger than $\mathcal{M}$ since it includes states, if any, whose recurrence orders are p; otherwise it is the same as $\mathcal{M}$. We will first show that

$$\limsup_{N \to \infty} \frac{1}{N} \sum_{t=1}^{N} \Pr(x(t) \in \bar{\mathcal{M}}) = 1. \tag{10}$$

Consider first the case $\rho > 0$. Clearly, $\rho = p$ or p^- for some $p \in \mathcal{R}$, where $p > 0$. Let

$$Q = \{q \in \mathcal{R}: \text{ for some } i \in \bar{\mathcal{M}}^c, \beta_i = q \text{ or } q^-\}.$$

Let $\theta = \inf_{q \in Q}(p - q)$, where $\inf \varnothing = +\infty$. Let

$$\gamma = \begin{cases} \theta & \text{if } \theta < +\infty, \\ p & \text{if } \theta = +\infty. \end{cases}$$

Consider the states in $\bar{\mathcal{M}}^c$ and observe that for sufficiently small $\delta > 0$,

$$\sum_{t=0}^{\infty} \Pr(x(t) \in \bar{\mathcal{M}}^c)\varepsilon(t)^{p-\gamma+\delta} < +\infty,$$

since the state space is finite. An application of Kronecker's Lemma (see Chung [6]) gives

$$\lim_{N \to \infty} \varepsilon(N)^{p-\gamma+\delta} \sum_{t=1}^{N} \Pr(x(t) \in \bar{\mathcal{M}}^c) = 0;$$

that is,

$$\lim_{N \to \infty} (N\varepsilon(N)^{p-\gamma+\delta}) \frac{1}{N} \sum_{t=1}^{N} \Pr(x(t) \in \bar{\mathcal{M}}^c) = 0. \tag{11}$$

Now we claim that

$$\limsup_{N \to \infty} N\varepsilon(N)^{p-\gamma+\delta} > 0. \tag{12}$$

Suppose not. Then,

$$\lim_{N \to \infty} N\varepsilon(N)^{p-\gamma+\delta} = 0,$$

and so

$$\lim_{N \to \infty} \frac{1/N}{\varepsilon(N)^{p-\gamma+\delta}} = +\infty.$$

In particular, we have

$$\lim_{N \to \infty} \left(\frac{1/N}{\varepsilon(N)^{p-\gamma+\delta}} \right)^{(p-\delta)/(p-\gamma+\delta)} = +\infty,$$

implying that

$$\lim_{N \to \infty} \frac{(1/N)^{(p-\delta)/(p-\gamma+\delta)}}{\varepsilon(N)^{p-\delta}} = +\infty.$$

However, since $\sum_{t=0}^{\infty} \varepsilon(t)^{p-\delta} = +\infty$, this would imply that

$$\sum_{N=1}^{\infty} \left(\frac{1}{N} \right)^{(p-\delta)/(p-\gamma+\delta)} = +\infty \quad \text{for all small } \delta > 0,$$

which is false. Hence, (12) holds and from (11) we deduce that

$$\liminf_{N \to \infty} \frac{1}{N} \sum_{t=1}^{N} \Pr(x(t) \in \bar{\mathcal{M}}^c) = 0. \tag{13}$$

But since

$$\frac{1}{N}\sum_{t=1}^{N}\Pr(x(t)\in\bar{\mathcal{M}})+\frac{1}{N}\sum_{t=1}^{N}\Pr(x(t)\in\bar{\mathcal{M}}^c)=1,$$

the result (10) follows.

Now turn to the case $\rho=0$. Then clearly, $\sum_{t=0}^{\infty}\Pr(x(t)\in\bar{\mathcal{M}}^c)<+\infty$, and so (13) is again true and the result (10) follows.

If $\rho=-\infty$, the result (10) is trivial.

To proceed from (10) to (9), it is clearly sufficient to show that in the case $\rho=p$ for some $p\in\mathcal{R}$, $p>0$,

$$\lim_{t\to\infty}\Pr(x(t)\in\{i:\beta_i=p^-\})=0.$$

This involves some results on the structure of the recurrence orders and is demonstrated in Lemma 5. □

Thus, knowledge of the recurrence orders $\{\beta_i\}$ provides knowledge about the asymptotic properties of the time-inhomogeneous Markov chain. In fact, as the reader may see from Example 1, the recurrence orders also provide information about the rates of convergence.

Our goal therefore is to determine the recurrence orders, and critical to that will be the following result established in [7], which shows that there is a fundamental balance of recurrence orders across every edge-cut in the graph of the Markov chain.

THEOREM 2 (Order Balance).

$$\max_{i\in A, j\in A^c}\beta_{ij}=\max_{i\in A, j\in A^c}\beta_{ji}\quad \textit{for every } A\subseteq X. \tag{14}$$

Equivalently, using the "⊖" notation and (7),

$$\max_{i\in A, j\in A^c}\beta_i\ominus V_{ij}=\max_{i\in A, j\in A^c}\beta_j\ominus V_{ji}\quad \textit{for every } A\subseteq X. \tag{15}$$

Proof. We sketch the proof; see [7] for the precise proof. Choose $A\subseteq X$ and note that if $\{\tau(n)\}_{n\geq 1}$ is the sequence of random times at which the process moves from A to A^c, while $\{\sigma(n)\}_{n\geq 1}$ is the sequence of random times at which the process moves from A^c back to A, then we have

$$\tau(n)<\sigma(n)<\tau(n+1),$$

where we have assumed, without loss of generality, that $x(0)\in A$ to give $\tau(1)<\sigma(1)$. Using this it follows from (5) that

$$\begin{aligned}
\sum_{t=0}^{+\infty}\varepsilon(t)^c I(x(t)\in A^c, x(t+1)\in A) &= \sum_{n=1}^{+\infty}\varepsilon(\sigma(n))^c\\
&\leqq M^c\sum_{n=1}^{+\infty}\varepsilon(\tau(n))^c\\
&= M^c\sum_{t=0}^{+\infty}\varepsilon(t)^c I(x(t)\in A, x(t+1)\in A^c)\\
&= M^c\sum_{n=1}^{+\infty}\varepsilon(\tau(n+1))^c + M^c\varepsilon(\tau(1))^c\\
&\leqq M^{2c}\sum_{n=1}^{+\infty}\varepsilon(\sigma(n))^c + M^{2c}\varepsilon(0)^c\\
&= M^{2c}\sum_{t=0}^{+\infty}\varepsilon(t)^c I(x(t)\in A^c, x(t+1)\in A) + M^{2c}\varepsilon(0)^c.
\end{aligned}$$

By taking expected values and using the Monotone Convergence Theorem, it follows that

$$\sum_{t=0}^{\infty} \varepsilon(t)^c \sum_{i\in A, j\in A^c} \pi_{ij}(t) < +\infty \Leftrightarrow \sum_{t=0}^{\infty} \varepsilon(t)^c \sum_{i\in A^c, j\in A} \pi_{ij}(t) < +\infty.$$

Hence both sides above converge or diverge together. Now if c is so large that every term on the left-hand side with $i\in A$, $j\in A^c$ converges, then clearly c is also so large that every term on the right-hand side converges. Thus,

$$c > \max_{i\in A, j\in A^c} \beta_{ij} \Leftrightarrow c > \max_{i\in A, j\in A^c} \beta_{ji}.$$

Likewise if c is small enough so that some term on the left-hand side diverges, then c is also small enough so that some term on the right-hand side diverges, and so

$$c \leqq \max_{i\in A, j\in A^c} \beta_{ij} \Leftrightarrow c \leqq \max_{i\in A, j\in A^c} \beta_{ji}. \qquad \square$$

Note that through Theorems 1 and 2 we have converted the problem of determining the asymptotic properties of the time-inhomogeneous Markov chain into an *algebraic* problem of solving the balance equations (14). Note that (14) provides a maximum of $2^{|X|}$ equations, one for each edgecut.

3. The modified balance equations. Note that if $(\beta_1, \beta_2, \cdots, \beta_{|X|})$ satisfy (15), then $(\beta_1 - a, \beta_2 - a, \cdots, \beta_{|X|} - a)$ also satisfy (15) for every a, i.e., the solution set is *translation invariant.* Thus (8), which fixes the *maximum* of the β_i's, also needs to be taken into account.

However, (15), (8) together can *still* possess nonunique solutions for sufficiently small values of ρ. In this section, we will show how we can obtain *one* solution to (15), (8); in the next section we show how to obtain *all* solutions.

In cases where there is a unique solution to the order balance equations, the algorithm of this section gives an $O(|X|^3)$ algorithm for determining it, compared to the algorithm of § 4 for obtaining all solutions (in the nonunique case), which is exponential in $|X|$. Also, the results of this section are used in the analysis of the simulated annealing algorithm in § 5.

It is convenient to consider the following "modified" balance equations that, as we show in the sequel, always possess a unique solution. Given $\rho \geqq 0$ and $V_{ij} \geqq 0$ for $i, j = 1, \cdots, |X|$ with $i \neq j$, consider the problem of determining $\lambda := (\lambda_1, \cdots, \lambda_{|X|})$ such that

$$\max_{i\in A, j\in A^c} \lambda_i - V_{ij} = \max_{i\in A, j\in A^c} \lambda_j - V_{ji} \quad \text{for every } A \subseteq \{1, \cdots, |X|\}, \tag{16}$$

and

$$\max_i \lambda_i = \rho. \tag{17}$$

We call (16), (17) the "modified" balance equations. Observe that (16) differs from (15) in that the operation "$-$" is used in place of "$\ominus$." Also, the λ's can be negative in (16).

We have introduced the modified balance equations to avoid the difficulties in handling $-\infty$ that occur under the "$\ominus$" operation.

THEOREM 3 (Properties of Order Balance and Modified Balance Equations). (1) *If λ satisfies the modified balance equations for a given ρ and V, then β defined by*

$$\beta_i := \lambda_i \ominus 0 \tag{18}$$

satisfies the order balance equations (15), (8) *for the given ρ and V.*

(2) *For every given ρ and V, there exists a unique solution λ to the modified balance equations. Moreover, the solutions for different values of ρ are translates of each other.*

(3) *Whenever ρ is large enough, there exists a unique solution to the order balance equations* (15), (8). *These unique solutions are all translates of the solutions for the modified balance equations.*

Proof. Suppose that for a fixed ρ and V, there exist *two distinct* solutions β and $\hat{\beta}$ to the order balance equations. Define

$$A := \{k \in X : \hat{\beta}_k \leqq \beta_k\}.$$

Then we claim that

$$\max_{i \in A, j \in A^c} \beta_i \ominus V_{ij} = \max_{i \in A, j \in A^c} \beta_j \ominus V_{ji} = -\infty$$

and

$$\max_{i \in A, j \in A^c} \hat{\beta}_i \ominus V_{ij} = \max_{i \in A, j \in A^c} \hat{\beta}_j \ominus V_{ji} = -\infty.$$

We need only consider the case where $A \neq \varnothing$ and $A \neq X$ (otherwise the claim is trivially true), and let us suppose to the contrary that both expressions are nonnegative. Then

$$\max_{i \in A, j \in A^c} \hat{\beta}_i \ominus V_{ij} = \max_{i \in A, j \in A^c} \hat{\beta}_j \ominus V_{ji} > \max_{i \in A, j \in A^c} \beta_j \ominus V_{ji} = \max_{i \in A, j \in A^c} \beta_i \ominus V_{ij} \geqq \max_{i \in A, j \in A^c} \hat{\beta}_i \ominus V_{ij},$$

which is a contradiction. The other two cases follow similarly, and so the claim is true. This shows that solutions to the order balance equations do not differ arbitrarily; specifically, all the arcs that separate A from A^c are transient.

Hence in particular, whenever we can show that

$$\beta_i \ominus V_{ij} \geqq 0 \quad \text{for all } i, j, \text{ with } i \neq j, \text{ and } V_{ij} < +\infty, \tag{19}$$

there can only exist *one* solution to the order balance equations for the given (ρ, V).

Now we show that this is indeed the case when ρ is large, which will prove the first part of the assertion (3) above. Specifically, suppose now that $\rho \geqq 2 \sum_{i,j: V_{ij} < +\infty} V_{ij}$.

Let $i_0 \in X$ be a state with $\beta_{i_0} = \rho$. For arbitrary $s \in X$, let $(i^* = i_0, i_1, \cdots, i_p = s)$ be a path from i^* to s such that $V_{i_{k-1} i_k} < +\infty$ for $k = 1, \cdots, p$ and $i_k \neq i_m$ for $k \neq m$. Let $l(i) = \arg\min_j V_{ij}$. With $A = \{i_k\}$ and applying the Order Balance Theorem 2, it is easy to see that

$$\beta_{i_{k-1}} \ominus V_{i_{k-1} i_k} \leqq \beta_{i_k} \ominus V_{i_k, l(i_k)} = \max_{j \neq i_k} (\beta_{i_k} \ominus V_{i_k, j}). \tag{20}$$

To prove that $\beta_s \geqq \max_{i,j: V_{ij} < +\infty} V_{ij} < +\infty$, it is sufficient to show that for $k = 1, \cdots, p$, along the path from i^* to s,

$$\beta_{i_k} \geqq \beta_{i_0} - V_{i_0, i_1} + V_{i_1, l(i_1)} - V_{i_1, i_2} + V_{i_2, l(i_2)} - \cdots - V_{i_{k-1} i_k} + V_{i_k, l(i_k)}, \tag{21}$$

since $\beta_{i_0} = \rho \geqq 2 \sum_{i,j: V_{ij} < +\infty} V_{ij}$.

We prove (21) by induction. For $k = 1$, from (20) we see that

$$\beta_{i_0} \ominus V_{i_0, i_1} \leqq \beta_{i_1} \ominus V_{i_1, l(i_1)}. \tag{22}$$

Clearly, the left-hand side of (22) is nonnegative, implying that the right-hand side is also nonnegative. Thus, we can replace "$\ominus$" with "$-$" giving

$$\beta_{i_1} \geqq \beta_{i_0} - V_{i_0, i_1} + V_{i_1, l(i_1)}. \tag{23}$$

Now assume (21) holds for $k-1$. From (20) we have

$$\beta_{i_{k-1}} \ominus V_{i_{k-1} i_k} \leqq \beta_{i_k} \ominus V_{i_k, l(i_k)}. \tag{24}$$

The left-hand side of (24) is nonnegative and so

$$\begin{aligned}\beta_{i_k} &\geqq \beta_{i_{k-1}} - V_{i_{k-1},i_k} + V_{i_k,l(i_k)} \\ &\geqq \beta_{i_0} - V_{i_0,i_1} + V_{i_1,l(i_1)} - V_{i_1,i_2} + V_{i_2,l(i_2)} - \cdots - V_{i_{k-1},i_k} + V_{i_k,l(i_k)},\end{aligned}$$

which completes the induction proof. This proves (19), and therefore there exists a unique solution whenever ρ is large enough, which is the first half of assertion (3) above.

Moreover, for the large enough ρ specified earlier, due to (19), we have $\beta_i \ominus V_{ij} = \beta_i - V_{ij}$. Hence $\{\beta_i\}$ itself satisfies the modified balance equations. In fact, this solution is unique to the modified balance equations since, if λ is any other solution, then we can prove in a fashion similar to the above, that $\lambda_i \geqq V_{ij}$ for all $j \in N_i$, thus yielding that $\lambda_i \ominus V_{ij} = \lambda_i - V_{ij}$, which in turn proves that λ is yet another solution to the order balance equations, which is a contradiction.

Hence, at least for large enough values of ρ we have proved the existence of a unique solution to the modified balance equations. However, it is easy to see that if λ satisfies the modified equations for a given (ρ, V), then $\lambda - \delta$ satisfies the modified balance equations for $(\rho - \delta, V)$, thus proving the existence of a unique solution to the modified balance equations for *all* (ρ, V). This proves the assertion (2) as well as the second half of the assertion (3) above.

Now we turn to the proof of assertion (1) above. Let A be arbitrary, and let $\{\lambda_i\}$ be the solution of the modified balance equations, and define $\beta_i := \lambda_i \ominus 0$. Suppose

$$\max_{i \in A, j \in A^c} \lambda_i - V_{ij} < 0.$$

Then by (16) we also have

$$\max_{i \in A, j \in A^c} \lambda_j - V_{ji} < 0.$$

However, then for each $i \in A$ and $j \in A^c$,

$$\beta_i \leqq \lambda_i < V_{ij} \quad \text{and} \quad \beta_j \leqq \lambda_j < V_{ji}.$$

Hence,

$$\beta_i \ominus V_{ij} = -\infty \quad \text{and} \quad \beta_j \ominus V_{ji} = -\infty,$$

and so

$$\max_{i \in A, j \in A^c} \beta_i \ominus V_{ij} = \max_{i \in A, j \in A^c} \beta_j \ominus V_{ji},$$

thus satisfying the original order balance equations. If, however,

$$\max_{i \in A, j \in A^c} \lambda_i - V_{ij} = \delta \geqq 0,$$

then by (16)

$$\max_{i \in A, j \in A^c} \lambda_j - V_{ji} = \delta \geqq 0.$$

Suppose that $(i_1, j_1) \in A \times A^c$ and $(i_2, j_2) \in A^c \times A$ are such that

$$\lambda_{i_1} - V_{i_1,j_1} = \lambda_{j_2} - V_{j_2,i_2} = \delta.$$

Then since

$$\lambda_{i_1} = V_{i_1,j_1} + \delta \geqq 0 \quad \text{and} \quad \lambda_{j_2} = V_{j_2,i_2} + \delta \geqq 0$$

we have

$$\beta_{i_1} = \lambda_{i_1} \quad \text{and} \quad \beta_{j_2} = \lambda_{j_2},$$

and so

$$\beta_{i_1} - V_{i_1,j_1} = \beta_{j_2} - V_{j_2,i_2}.$$

Also, since $\lambda_k \geqq \beta_k$, we have

$$\begin{aligned}\max_{i\in A, j\in A'} \beta_i \ominus V_{i,j} &\leqq \max_{i\in A, j\in A'} \lambda_i \ominus V_{ij} \\ &\leqq \max_{i\in A, j\in A'} \lambda_i - V_{ij} \\ &= \lambda_{i_1} - V_{i_1,j_1} \\ &= \beta_{i_1} - V_{i_1,j_1} \\ &= \beta_{i_1} \ominus V_{i_1,j_1}.\end{aligned}$$

Similarly, $\max_{i\in A, j\in A'} \beta_j \ominus V_{ji} = \beta_{j_2} \ominus V_{j_2,i_2}$, and so

$$\max_{i\in A, j\in A'} \beta_i \ominus V_{ij} = \max_{i\in A, j\in A'} \beta_j \ominus V_{ji}.$$

This proves the assertion (1) and the theorem. □

Remark 1. It is interesting to note that the existence of a solution to the modified balance equations has been proved by relying on the existence of a solution to the order balance equations, which in turn is guaranteed by the probabilistic arguments of Theorem 2. A separate independent constructive proof of existence, which does not use probabilistic arguments, can be found in [8].

We now give an algorithm for determining the *unique* solution to the modified balance equations. An illustrative example is convenient.

Example 2. Let $\rho = 5$ and

$$V = [V_{ij}] = \begin{Bmatrix} \bigstar & 4 & 3 & 1 \\ 6 & \bigstar & 3 & 7 \\ 6 & 2 & \bigstar & 4 \\ 2 & 6 & 5 & \bigstar \end{Bmatrix}.$$

Our goal is to determine $\lambda = (\lambda_1, \cdots, \lambda_4)$, which satisfies (16), (17). We shall refer to $\lambda_i - V_{ij}$ as the λ-*flow* along the arc (i, j). Consider first the modified balance equation for the edge cut $A = \{i\}$,

$$\max_{j\neq i} \lambda_i - V_{ij} = \max_{j\neq i} \lambda_j - V_{ji}. \tag{25}$$

Observe that the left-hand side of (25) can be written as

$$\lambda_i - \min_{j\neq i} V_{ij},$$

and so the arc of *maximum* λ-*flow* out of $A = \{i\}$ is the arc $(i, l(i))$ where

$$l(i) = \arg\min_{j\neq i} V_{ij}.$$

(Note that $l(i)$ may not be unique.)

We now construct the directed graph $G_1 = (V_1, E_1)$, with $V_1 = \{\{1\}, \cdots, \{4\}\}$ and $(i, j) \in E_1$ if $j = l(i)$. See Fig. 1.

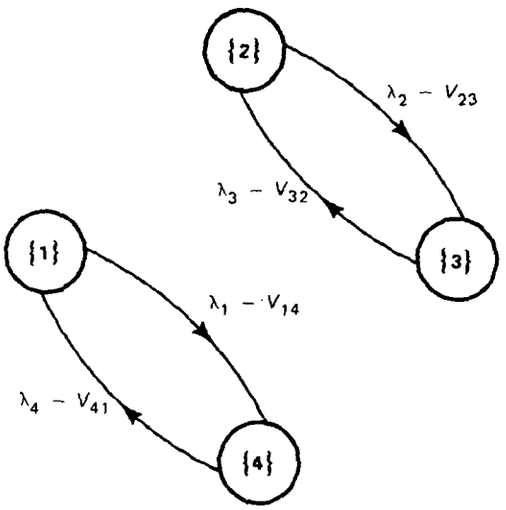

FIG. 1. *The graph G_1 of Example 2.*

Note that G_1 has two directed cycles $\{1\}\to\{4\}\to\{1\}$ and $\{2\}\to\{3\}\to\{2\}$. Let us examine the λ-flows on the directed cycle $\{1\}\to\{4\}\to\{1\}$. Since $\lambda_1 - V_{14}$ is the maximum λ-flow out of $\{1\}$, it is not smaller than any λ-flow into $\{1\}$, and so in particular

$$\lambda_1 - V_{14} \geqq \lambda_4 - V_{41}.$$

Also, $\lambda_4 - V_{41}$ is the maximum λ-flow out of $\{4\}$ and so

$$\lambda_4 - V_{41} \geqq \lambda_1 - V_{14}.$$

We thus observe that the λ-flows along the directed cycle $\{1\}\to\{4\}\to\{1\}$ are *equal*; that is,

$$\lambda_1 - V_{14} = \lambda_4 - V_{41},$$

and so

$$\lambda_1 - 1 = \lambda_4 - 2. \tag{26}$$

Thus, we have determined the *difference* between λ_1 and λ_4.

In exactly the same way, from the directed cycle $\{2\}\to\{3\}\to\{2\}$ we see that

$$\lambda_2 - 3 = \lambda_3 - 2, \tag{27}$$

thus determining the difference between λ_2 and λ_3.

At the next step of the algorithm, consider the modified balance equations for the edge cut (A, A^c) where $A = \{1, 4\}$ and $A^c = \{2, 3\}$. Observe that for $A = \{1, 4\}$, the left-hand side of the modified balance equation

$$\max_{i\in A, j\in A^c} \lambda_i - V_{ij} = \max_{i\in A, j\in A^c} \lambda_j - V_{ji} \tag{28}$$

can be written as

$$\max(\lambda_1 - V_{12}, \lambda_1 - V_{13}, \lambda_4 - V_{42}, \lambda_4 - V_{43});$$

that is,

$$\max(\lambda_1 - 4, \lambda_1 - 3, \lambda_4 - 6, \lambda_4 - 5).$$

We have previously determined that $\lambda_4 - \lambda_1 = 1$, and so the maximum is achieved by $\lambda_1 - V_{13} = \lambda_1 - 3$, and the arc of maximum λ-flow out of $\{1, 4\}$ is the arc $(1, 3)$.

In a similar fashion, examining the right-hand side of the modified balance equation (28), we determine that the maximum λ-flow out of $\{2, 3\}$ is achieved by $\lambda_3 - V_{34} = \lambda_3 - 4$, and so the arc of maximum λ-flow out of $\{2, 3\}$ is $(3, 4)$.

We now consider the directed graph $G_2 = (V_2, E_2)$, with $V_2 = \{\{1, 4\}, \{2, 3\}\}$ and $E_2 = \{(1, 3), (3, 4)\}$ shown in Fig. 2. Note that E_2 is the set of the arcs of maximum λ-flow out of the edge cuts in V_2.

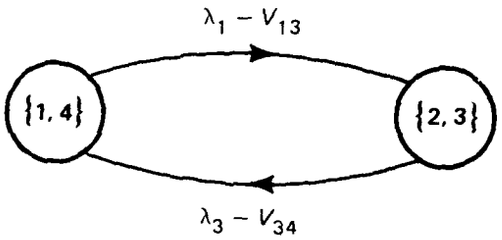

FIG. 2. *The graph G_2 of Example 2.*

Observe that G_2 has a directed cycle $\{1, 4\} \to \{2, 3\} \to \{1, 4\}$. Now note that $\lambda_1 - V_{13}$ is the maximum λ-flow out of $\{1, 4\}$ and $\lambda_3 - V_{34}$ is the maximum λ-flow out of $\{2, 3\}$ and so

$$\lambda_1 - V_{13} = \lambda_3 - V_{34};$$

that is,

$$\lambda_1 - 3 = \lambda_3 - 4. \tag{29}$$

Combining (26), (27), and (29), we obtain

$$\lambda_1 - 3 = \lambda_2 - 5 = \lambda_3 - 4 = \lambda_4 - 4. \tag{30}$$

We now know the *pairwise differences* between *all* of the λ_i's, and so we do not need to consider any additional edge cuts. To fix the values of $\{\lambda_i\}$, we use the value of ρ to give

$$\max_{i \in X} \lambda_i = \rho = 5.$$

Since, from (30), λ_2 is the largest, we set $\lambda_2 = 5$. We thus obtain the solution to the modified balance equations:

$$\lambda_1 = 3, \quad \lambda_2 = 5, \quad \lambda_3 = \lambda_4 = 4.$$

The principal idea used to solve the modified balance equations in Example 2 is summarized in the following lemma.

LEMMA 2. (1) *Given $A \subseteq X$ for which we know the pairwise differences between all the λ_i's for states in A, we can determine the arc of maximum λ-flow out of A (without knowing the λ_i's themselves).*

(2) *Let $A_1, A_2, \cdots, A_p$ be a partition of X and suppose for each A_k we know all the pairwise differences between the λ_i's for all states in A_k. Let (i_k, j_k) denote the arc of maximum λ-flow out of A_k. Construct the directed graph $G = (V, E)$, with $V = \{A_1, \cdots, A_p\}$ and $E = \{(i_1, j_1), \cdots, (i_p, j_p)\}$. There exists a directed cycle on G. If*

$\{A_{n_1}, \cdots, A_{n_m}\}$ is the list of vertices, in order, along the directed cycle, then the λ-flow on the directed cycle is constant; that is,

$$\lambda_{i_{n_1}} - V_{i_{n_1}, j_{n_1}} = \cdots = \lambda_{i_{n_m}} - V_{i_{n_m}, j_{n_m}},$$

and we can determine the pairwise differences between the values of the λ_i's for all the states in $\bigcup_{k=1}^{m} A_{n_k}$.

Proof. (1) Without loss of generality, suppose A is the set of states $\{1, 2, \cdots, r\}$. Let $\alpha_i := \lambda_1 - \lambda_i$. (We know the α_i's.) Then

$$\max_{i \in A, j \in A^c} \lambda_i - V_{ij} = \max_{i \in A, j \in A^c} \lambda_1 - \alpha_i - V_{ij} = \lambda_1 - \min_{i \in A, j \in A^c} (\alpha_i + V_{ij}).$$

Thus, the arc

$$(i^*, j^*) := \arg \min_{i \in A, j \in A^c} (\alpha_i + V_{ij})$$

is an arc of maximum λ-flow out of A.

(2) The out-degree of each vertex of G is at least one, and so from elementary graph theory it follows that G has a directed cycle. Suppose

$$A_{n_1} \to A_{n_2} \to \cdots \to A_{n_m} \to A_{n_1}$$

is such a directed cycle. Then we have the situation shown in Fig. 3. Now (i_{n_k}, j_{n_k}) is the arc of maximum λ-flow *out* of A_{n_k}, and so the λ-flow on this arc is not less than the λ-flow of any arc *into* A_{n_k}. In particular,

$$\lambda_{i_{n_k}} - V_{i_{n_k}, j_{n_k}} \geqq \lambda_{i_{n_{k-1}}, j_{n_{k-1}}} - V_{i_{n_{k-1}}, j_{n_{k-1}}} \quad \text{for } k = 1, \cdots, m,$$

where, for convenience, we implicitly identify i_{n_0} with i_{n_m} and j_{n_0} with j_{n_m}. Thus,

$$\begin{aligned}
\lambda_{i_{n_m}} - V_{i_{n_m}, j_{n_m}} &\geqq \lambda_{i_{n_{m-1}}} - V_{i_{n_{m-1}}, j_{n_{m-1}}} \\
&\geqq \lambda_{i_{n_{m-2}}} - V_{i_{n_{m-2}}, j_{n_{m-2}}} \\
&\vdots \\
&\geqq \lambda_{i_{n_1}} - V_{i_{n_1}, j_{n_1}} \\
&\geqq \lambda_{i_{n_m}} - V_{i_{n_m}, j_{n_m}}.
\end{aligned}$$

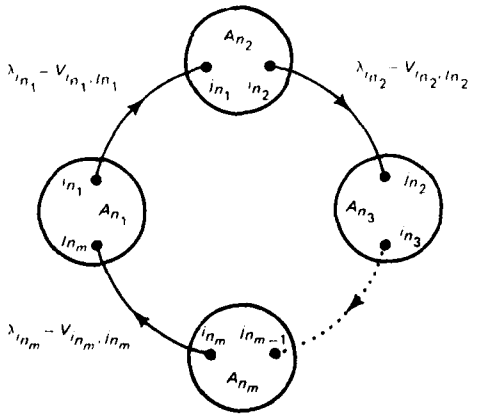

FIG. 3. *A directed cycle of maximum λ-flows in Lemma 3.*

Therefore, the λ-flow on the directed cycle is a constant:

$$\lambda_{i_{n_1}} - V_{i_{n_1} j_{n_1}} = \lambda_{i_{n_2}} - V_{i_{n_2} j_{n_2}} = \cdots = \lambda_{i_{n_m}} - V_{i_{n_m} j_{n_m}}. \tag{31}$$

For each A_{n_k} in the directed cycle, we know the pairwise differences between the λ_i's for states in A_{n_k}. Using (31) we can now easily determine the pairwise differences between all the λ_i's for states in $\cup_{k=1}^{m} A_{n_k}$. □

The algorithm for solving the modified balance equations is outlined below.

ALGORITHM TO SOLVE MODIFIED BALANCE EQUATIONS.

Step 1. Set $A_i^1 = \{i\}$ for $i = 1, \cdots, |X|$. We call the A_i^k's *coalitions at step k*. Note that for every i, the pairwise differences between the λ-values for all states in A_i^1 are (trivially) known. Set $A^1 := \{A_1^1, A_2^1, \cdots, A_{|X|}^1\}$. Let $N(1) = |A^1| =:$ the number of elements in the set A^1 = number of coalitions at Step 1.

Step k. Given $A^k := \{A_1^k, A_2^k, \cdots, A_{N(k)}^k\}$, where for each $A_j^k \in A^k$ the pairwise differences between all of the λ_i's for i's in A_j^k are known, construct A^{k+1} as follows. Using Lemma 2, identify the directed cycles in the graph. (There exists at least one directed cycle.) The elements of A^{k+1} consist of the directed cycles identified in the graph, and those $A_j^k \in A^k$ that are not in any directed cycle. (More precisely, if $\{A_{n_1}^k, A_{n_2}^k, \cdots, A_{n_m}^k\}$ is a directed cycle, then $\cup_{i=1}^{m} A_{n_i}$ is an element of A^{k+1}.) Note that for every $A_j^{k+1} \in A^{k+1}$, the pairwise differences between all of the λ_i's for i's in A_j^{k+1} are known. Furthermore, if $N(k) := |A^k|$, then $N(k+1) < N(k)$.

Last Step. Stop when $N(k) = 1$. Note that the pairwise differences between *all* λ_i's are known, and the λ satisfying the modified balance equations can be obtained by a translation by using the given value of ρ. □

4. An algorithm to obtain all solutions of the order balance equations. We now characterize *all* solutions to the order balance equations, and describe an algorithm for generating *all* these solutions. To do so we will use the coalitions $\{A_i^k\}$ generated by the algorithm of the preceding section. Let us call $\lambda_i - V_{ij}$ and $\beta_{ij} = \beta_i \ominus V_{ij}$ as the *λ-flow* and *β-flow*, respectively, along the arc (i, j).

LEMMA 3. (1) *If (i, j) is an arc of maximum λ-flow out of A_l^k, then it is also an arc of maximum β-flow out of A_l^k.*

(2) *If $\{A_1^k, \cdots, A_p^k\}$ is a directed cycle obtained at step k, then the β-flow along the directed cycle is a constant.*

(3) *If the β-flow along the directed cycle $\{A_1^k, \cdots, A_p^k\}$ obtained at step k is $-\infty$, then the β-flow along any directed cycle obtained at step $n > k$ containing $A_l^n = \cup_{i=1}^{p_n} A_i^k$ as a node, is also $-\infty$.*

(4) *If the β-flow along the directed cycle $\{A_1^k, \cdots, A_p^k\}$ obtained at step k is $\geqq 0$, then for every $i, j \in A_l^{k+1} := \cup_{m=1}^{p_{k+1}} A_m^k$ there exists a path $(i = i_0, i_1, \cdots, i_q = j)$ such that $i_m \in A_l^{k+1}$ and $\beta_{i_m, i_{m+1}} \geqq 0$ for $0 \leqq m \leqq q-1$.*

Proof. We will first prove (1)-(3) by induction. Consider $k = 1$. Since A_l^k is then just a singleton, say $A_l^k = \{l\}$, an arc (l, m) of maximum λ-flow out of $\{l\}$ is just one for which $V_{lm} = \min_n V_{ln}$. Clearly this is also an arc for which $\beta_l \ominus V_{lm} = \min_n \beta_l \ominus V_{ln}$. Now suppose that $\{A_1^k, \cdots, A_p^k\}$ is a directed cycle of such maximum flows. Then an application of the Order Balance Theorem to each A_l^k shows that $\beta_{12} = \beta_{23} = \cdots = \beta_{p1}$. Suppose now that $\beta_{12} = \beta_{23} = \cdots = \beta_{p1} = -\infty$. Then if (l, m) is an arc of maximum β-flow out of $\cup_{i=1}^{p} A_i^k$, clearly $\beta_{lm} \leqq \beta_{l,l+1} = -\infty$. Thus the assertion is true for $k = 1$.

Now suppose that the assertion is true for $1, 2, \cdots, k-1$. Consider a coalition A_l^k. If the β-flow along some directed cycle $\{A_1^n, \cdots, A_q^n\}$ at some step $n < k$ with $A_l^k = \cup_{i=1}^{q} A_i^n$ was $-\infty$, then clearly the maximum β-flow out of A_l^k is $-\infty$, and so *any*

arc out of A_l^k is an arc of maximum β-flow. On the other hand if the β-flow along the directed cycle $\{A_1^n, \cdots, A_q^n\}$ is $\geqq 0$, then the differences between the β_i's for states $i \in A_l^k$ are the *same* as the differences between the λ_i's, i.e.,

$$\beta_i - \beta_j = \lambda_i - \lambda_j \quad \text{for all } i, j \in A_l^k, \tag{32}$$

and so the arc of maximum λ-flow out from A_l^k is also an arc of maximum β-flow out from A_l^k. Moreover, if $\{A_1^k, \cdots, A_p^k\}$ is a directed cycle at step k, then an application of the Order Balance Theorem to each A_l^k shows that the β-flow along the directed cycle is a constant. Finally, if this β-flow is $-\infty$, suppose that (r, m) is a maximum flow arc out of $\cup_{l=1}^p A_l^k$. Suppose that $r \in A_l^k$. Then clearly $\max_{i \in A_l^k, j \in A_l^c} \beta_{ij} \geqq \beta_{rm}$ and so $\beta_{rm} = -\infty$. This completes the induction and the proof.

Finally, to see (4), note first that from (1), (2), and (3), the β-flow along any directed cycles contained within A_l^{k+1} is $\geqq 0$. Since A_l^{k+1} is formed as the union of such directed cycles, the result follows. □

Motivated by (3) and (4) above, we introduce the following definition.

DEFINITION 4. We shall say that i is *recurrently connected* to j if there exists a path $(i = i_0, i_1, \cdots, i_q = j)$ with $\beta_{i_m, i_{m+1}} \geqq 0$ for $0 \leqq m \leqq q-1$.

We shall say that a set $A \subseteq X$ is a *recurrently connected set* if for every $i, j \in A$ and $k \in A^c$, i is recurrently connected to j but not to k.

From Lemma 3 it follows that recurrently connected sets are precisely those A_l^k's for which the β-flow out of A_l^k is $-\infty$, while the β-flows along the directed cycles contained within A_l^k are $\geqq 0$. Note also that the recurrently connected sets form a *partition* of X.

We now proceed to determine which sets are possible candidates for being recurrently connected sets. Consider a typical candidate A_l^{k+1}. Let $\mathcal{F}$ denote the β-flow on the cycle $\{A_1^k, \cdots, A_p^k\}$, where $A_l^{k+1} = \cup_{l=1}^p A_l^k$. Then if (i_m, j_m) is the arc of maximum flow out of A_m^k (and, by construction, into $A_{(m+1) \bmod p}^k$), we must have

$$\mathcal{F} = \beta_{i_1} - V_{i_1, j_1} = \beta_{i_2} - V_{i_2, j_2} = \cdots = \beta_{i_p} - V_{i_p, j_p} \geqq 0,$$

$$\max_{i \in A_l^{k+1}, j \notin A_l^{k+1}} \beta_i - V_{ij} < 0, \quad \max_{i \in A_l^{k+1}} \beta_i \leqq \rho.$$

We will now attempt to determine whether there exist $\{\beta_i : i \in A_l^{k+1}\}$ that satisfy these conditions. Note that if this is not feasible, then A_l^{k+1} cannot be a recurrently connected set.

Let (x, y) denote the arc of maximum β-flow out of A_l^{k+1}. Then $\beta_x < V_{xy}$. Fix m to be an arbitrarily chosen state from A_l^{k+1}. Then for every state $h \in A_l^{k+1}$ we know the value of $(\beta_h - \beta_m)$ from Lemma 3 above. Let us define

$$\zeta_h := \beta_h - \beta_m.$$

Then

$$\begin{aligned} \mathcal{F} &= \beta_{i_1} - V_{i_1, j_1} \\ &= \beta_m + \zeta_{i_1} - V_{i_1, j_1} \\ &= \beta_x - \zeta_x + \zeta_{i_1} - V_{i_1, j_1} \\ &< V_{xy} - \zeta_x + \zeta_{i_1} - V_{i_1, j_1} =: M_1, \end{aligned}$$

giving an upper bound on $\mathcal{F}$.

We must also satisfy the constraint $\max_{i \in A_l^{k+1}} \beta_i \leqq \rho$, and so let

$$\theta := \arg \max_{i \in A_l^{k+1}} \zeta_i.$$

Then it is clear that $\beta_\theta \geqq \max_{i \in A_l^{k+1}} \beta_i$. Thus,

$$\begin{aligned}\rho &\geqq \beta_\theta \\ &= \beta_m + \zeta_\theta \\ &= \beta_{i_1} - \zeta_{i_1} + \zeta_\theta \\ &= \beta_{i_1} - V_{i_1,j_1} + V_{i_1,j_1} - \zeta_{i_1} + \zeta_\theta \\ &= \mathscr{F} + V_{i_1,j_1} - \zeta_{i_1} + \zeta_\theta,\end{aligned}$$

and so

$$\mathscr{F} \leqq \rho - V_{i_1,j_1} + \zeta_{i_1} - \zeta_\theta =: M_2,$$

giving yet another upper bound on $\mathscr{F}$. (Note. If $A_l^{k+1} = \{i\}$, then $M_1 = \min_j V_{ij}$ and $M_2 = \rho$.)

Any choice of $\mathscr{F}$ from the interval

$$\Omega(A_l^{k+1}) := [0, M_1) \cap [0, M_2]$$

will allow assignments for the recurrence orders of states in A_l^{k+1} consistent with the assumption that the coalition A_l^{k+1} is a recurrently connected set. If $\Omega(A_l^{k+1}) = \varnothing$ then then there is no assignment, and so A_l^{k+1} is not a recurrently connected set.

We still need to determine the set of all recurrently connected sets. To do this we construct a *rooted tree* having the coalitions produced by the general procedure as nodes, and having a directed edge from coalition A_p^{k+1} to A_r^k if $A_p^{k+1} \supseteq A_r^{(k)}$. Hence, the root of the tree is X, and its leaves are the singleton sets $\{1\}, \{2\}, \cdots, \{n\}$. Let D_i be the set of the leaves of the tree that are *descendants* of the node i in the rooted tree.

We say that a set Ξ of nodes is a *proper cover* if

$$\bigcup_{A \in \Xi} D_A = X$$

and

$$D_A \cap D_{A'} = \varnothing \quad \text{for } A \neq A'.$$

Now the algorithm to determine all the solutions of (15), (8) proceeds as follows. Let a set $\Xi := \{A_1, A_2, \cdots, A_k\}$ be a proper cover. Now we will determine whether Ξ can be a set of *all* recurrently connected sets, as follows. First we determine $\Omega(A_j)$ for every $A_j \in \Xi$. (Note that if we guess X to be a recurrently connected set, then $\Omega(X) = [0, M_2]$, since the M_1 upper bound is $+\infty$ because there is no maximal flow out of X. Also, if we guess the singleton $\{i\}$ to be a recurrently connected set, then $\Omega(\{i\}) = -\infty \cup ([0, M_1) \cap [0, M_2])$. If *any* of the $\Omega(A_j)$'s is empty, then the guess Ξ is *not* a feasible set of recurrently connected sets. If *every* $\Omega(A_j)$ is nonempty, then let $\bar{\mathscr{F}}_j := \sup \Omega(A_j)$. If this "sup" is not attained, then we cannot assign ρ to any state in A_j. If this "sup" is attained, then we determine for each such A_j whether, with the choice of $\bar{\mathscr{F}}_j$, there is a state $i_j \in A_j$ with $\beta_{i_j} = \rho$. If no such state exists for *any* A_j, then again Ξ is *not* a feasible set of recurrently connected sets. Finally, if there exist such A_j's then let $\mathscr{A}(\Xi)$ be the set of all such A_j's. Now, the set of all solutions corresponding to Ξ is obtained by picking, in turn, an A_j from $\mathscr{A}(\Xi)$, fixing its flow as $\bar{\mathscr{F}}_j$, and choosing all other $\mathscr{F}_j$'s arbitrarily from the $\Omega(A_j)$'s. By checking *every* proper cover Ξ, we thus determine all solutions to the order balance equations, as the following theorem shows.

THEOREM 4. *All solutions to the order balance equations can be generated by using the method described above.*

Proof. Suppose β satisfies the order balance equations. Then for this solution determine the set Ξ of recurrently connected sets. This set must be a proper cover. For this set Ξ, there must be some A_j with corresponding β-flow equal $\bar{\mathcal{F}}_j$. Now determine the β-flows on the recurrently connected sets. We generate this solution β when we choose Ξ as the set of recurrently connected sets, and A_j as the coalition with maximum flow equal to $\bar{\mathcal{F}}_j$, and assign the correct β-flows on the other recurrently connected sets. □

This algorithm takes an exponential in $|X|$ number of steps, due to the necessity of checking all proper covers. However, the complexity issue is not the primary concern here, since the problem of asymptotic analysis of the stochastic process is not a priori known to be a problem resolvable by a finite algorithm.

We illustrate the procedure for determining all solutions to the order balance equations.

Example 3. We construct all solutions to the order balance equations for Example 2 when $\rho = 4$. See Fig. 4 for the rooted tree. We check the proper covers:

(1) $\Xi = \{X\}$: $\Omega(X)$ is empty, so X cannot be a recurrently connected set.

(2) $\Xi = \{\{1, 4\}, \{2, 3\}\}$: Using the method described above we obtain

$$\beta_1 = \alpha, \quad \beta_2 = 4, \quad \beta_3 = 3, \quad \beta_4 = 1 + \alpha$$

where $1 \leqq \alpha < 3$.

(3) $\Xi = \{\{1, 4\}, \{2\}, \{3\}\}$: $\max_{i \in X} \beta_i < 4$, a contradiction.

(4) $\Xi = \{\{1\}, \{4\}, \{2, 3\}\}$:

$$\beta_1 = \gamma, \quad \beta_2 = 4, \quad \beta_3 = 3, \quad \beta_4 = \theta$$

where $\gamma = -\infty$ or $0 \leqq \gamma < 1$, and $\theta = -\infty$ or $0 \leqq \theta < 2$.

(5) $\Xi = \{\{1\}, \{2\}, \{3\}, \{4\}\}$: $\max_{i \in X} \beta_i < 4$, and so $\{\{1\}, \{2\}, \{3\}, \{4\}\}$ is not a set of recurrently connected sets.

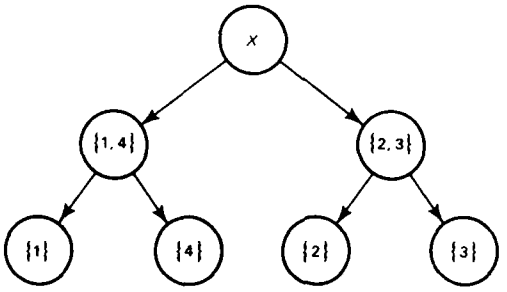

FIG. 4. *The rooted tree of Example* 3.

We have checked all proper covers. Hence the set of all solutions is $\{(\alpha, 4, 3, 1 + \alpha): 1 \leqq \alpha < 3\} \cup \{(\gamma, 4, 3, \theta): \gamma = -\infty \text{ or } 0 \leqq \gamma < 1 \text{ and } \theta = -\infty \text{ or } 0 \leqq \theta < 2\}$.

How can nonunique solutions to the order balance equations arise, and what is the implication of such nonuniqueness? First let us consider the case where a unique solution exists. Since such a solution is uniquely determined by the algorithm, it is clear that the recurrence orders of the states, and thus the rates of convergence of the transition probabilities, depend only on the V_{ij}'s in the transition probabilities $p_{ij}(t) = c_{ij}\epsilon(t)^{V_{ij}}$, and *not* on the proportionality constants $\{c_{ij}\}$. However, in the case of *nonunique* solutions, the following example shows that the recurrence orders may even depend on the *proportionality constants* $\{c_{ij}\}$.

Example 4. Let $X = \{1, 2, 3\}$ and $V_{ij} = \max\{0, j - i\}$. Let $c_{13} = c_{23} = 1$, $c_{31} = 1 - \alpha$, and $c_{32} = \alpha$, where $\alpha \in (0, 1)$. Set $c_{ij} = 0$ for all other i, j. See Fig. 5. Let the cooling schedule be $\epsilon(t) = 1/t$. Then the *complete* set of order balance equations obtained by using *all* edge cuts is:

$$\beta_2 \ominus V_{23} = \beta_3 \ominus V_{32}, \qquad \beta_3 \ominus V_{31} = \beta_1 \ominus V_{13},$$

$$\max(\beta_2 \ominus V_{23}, \beta_1 \ominus V_{13}) = \max(\beta_3 \ominus V_{32}, \beta_3 \ominus V_{31}),$$

with the maximum given by,

$$\max_{i \in X} \beta_i = 1.$$

The assignments

$$\beta_1 = 1, \quad \beta_2 = \gamma, \quad \beta_3 = -\infty$$

satisfy the order balance equations for *every* $\gamma \in \{-\infty\} \cup [0, 1)$. Thus any value of $\beta_2 < 1$ *gives a solution of the order balance equations.*

However, a calculation that can be found in [8] shows that the correct order of recurrence of state 2 is

$$\beta_2 = \alpha.$$

Thus, the order of recurrence, and the rate of convergence of the probability $\Pr(x(t) = 2)$ to zero, depends on the proportionality constant $c_{32} = \alpha$ involved.

Based on the above results, we obtain the following property of the orders of recurrence of the states in a recurrently connected set.

LEMMA 4. *Consider a recurrently connected set A.*

(1) *If* $\beta_i \in \mathcal{R}$ *for some* $i \in A$, *then* $\beta_j \in \mathcal{R}$ *for all* $j \in A$.

(2) *If for some* $i \in A$, $\beta_i = p_i$ *for some* $p_i \in \mathcal{R}$, *then for every* $j \in A$, $\beta_j = p_j$ *for some* $p_j \in \mathcal{R}$.

Proof. The proof follows immediately from (32). □

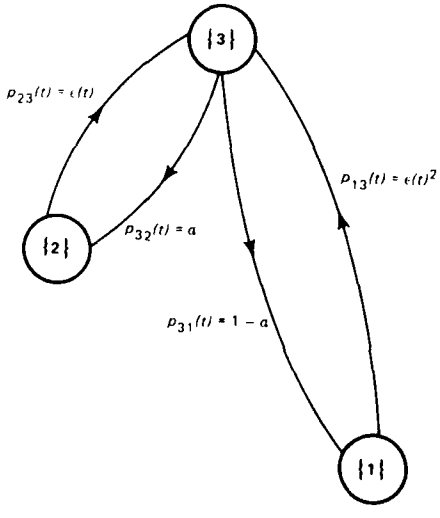

FIG. 5. *The Markov process of Example* 4.

Thus all recurrence orders in a recurrently connected set are of the same type, i.e., either they are all real numbers p_i, or they are all of the type p_i^-, or they are all $-\infty$ (see Definition 1).

This gives us the following lemma, which completes the proof of Theorem 1.

LEMMA 5. *Suppose the rate of cooling is $\rho = p \in \mathcal{R}$, with $p > 0$, i.e., the maximum is achieved in Definition* 3. *If there is a state $i \in X$ for which $\beta_i = p^-$, then* $\lim_{t\to\infty} \Pr(x(t) = i) = 0$.

Proof. Suppose A is the recurrently connected class to which i belongs. Since all arcs *between* recurrently connected sets are transient, it follows from the Borel-Cantelli Lemma that along almost every sample path ω there can only be a *finite* number of transitions between different recurrently connected sets. Hence for almost every ω, $\{x(t, \omega)\}$ converges to some recurrently connected set. Hence the limit $\lim_{t\to\infty} \Pr(x(t) \in A)$ exists. Now we show that this limit is zero. Suppose not, i.e., suppose $\lim_{t\to\infty} \sum_{j\in A} \pi_j(t) = \delta > 0$. Then it follows that $\sum_{t=0}^{\infty} \varepsilon(t)^p \sum_{j\in A} \pi_i(t) = +\infty$. Hence for some $j \in A$, $\beta_j = p$. But then by Lemma 4, $\beta_i \in \mathcal{R}$, which gives a contradiction. □

5. Weak reversibility and simulated annealing. We now turn our attention to the special class of Markov chains arising from the method of *optimization by simulated annealing*. Recall that the Markov chains in this class satisfy (1)-(6) with the special choice of

$$V_{ij} := \max\{0, W_j - W_i\}.$$

In [7] it was shown that under the "symmetric neighborhood" assumption, $c_{ij} > 0$ if and only if $c_{ji} > 0$, the orders of recurrence satisfy the following *detailed order balance*:

$$\beta_{ij} = \beta_{ji} \quad \text{for every } i, j \in X.$$

It is easy to see that the detailed order balance above is equivalent to the sum of the order of recurrence of a state and its cost being constant on recurrently connected sets.

In this section we will show that this constancy property of the sum of the recurrence order and cost on recurrently connected sets continues to hold under the much weaker assumption of "weak reversibility" introduced by Hajek in [1].

DEFINITION 5. A state i is said to be reachable from state j if there is a sequence of states $j = i_0, i_1, \cdots, i_p = i$ such that $c_{i_k, i_{k+1}} > 0$ for $0 \leqq k \leqq p-1$.

DEFINITION 6. A state i is reachable at height H from j if there is a path from j to i as in Definition 5 for which $W_{i_k} \leqq H$ for $0 \leqq k \leqq p$.

ASSUMPTION 1(Weak Reversibility). For any real number H and any two states i and j, i is reachable at height H from j if and only if j is reachable at height H from i.

In what follows we assume weak reversibility.

THEOREM 5 (The Potential Theorem). *Under Assumption* 1, *for every recurrently connected set A there exists a constant $\alpha(A)$ such that $\beta_i + W_i = \alpha(A)$ for every $i \in A$.*

Proof. We fix our attention on a particular recurrently connected set A. Assume to the contrary that A can be partitioned into *equipotential* sets $C_1, C_2, \cdots, C_r$ such that $\beta_i + W_i = \alpha(C_k)$ for every $i \in C_k$, where the $\alpha(C_k)$'s are distinct constants. We will show that there is only one equipotential set, namely, A.

For each equipotential set C_i, determine an arc of maximum β-flow out of the set. From Lemma 2, there exists a directed cycle of these equipotential sets, and the β-flow along the directed cycle is constant. Moreover, from Lemma 3, since A is a recurrently connected set, these β-flows are all nonnegative. Without loss of generality, label the sets along the directed cycle $C_1, C_2, \cdots, C_p$ such that the constant $\alpha(C_1)$ associated with the set C_1 is smallest. Let (i_s, j_s) be the arc of maximum β-flow out

of the set C_s. By construction, $i_s \in C_s$ and $j_s \in C_{(1+s) \bmod p}$ and

$$\beta_{i_1,j_1} = \beta_{i_2,j_2} = \cdots = \beta_{i_p,j_p} \geqq 0.$$

Knowing that $\beta_{i_1,j_1} \geqq 0$ we consider the two cases: (1) $W_{j_1} \geqq W_{i_1}$; or (2) $W_{j_1} < W_{i_1}$.

If case (1) is true then since j_1 is reachable at height W_{j_1} from i_1, by the weak reversibility assumption there exists a path from j_1 back to i_1 that does not go through any states with costs larger than W_{j_1}. Let (k, l) be the particular arc of that path that exits C_2. Note that

$$\begin{aligned}\beta_{i_1,j_1} &= \beta_{i_2,j_2} \\ &\geqq \beta_{kl},\end{aligned}$$

because β_{i_2,j_2} is the arc of maximum β-flow out of C_2. If $\beta_{kl} \geqq 0$ then $\beta_{kl} = \beta_k + W_k - W_l$. If $\beta_{kl} < 0$ then $\beta_k + W_k - W_l < 0$. In either case, since $\beta_{i_1,j_1} \geqq 0$, we have that

$$\beta_{i_1,j_1} = \beta_{i_1} + W_{i_1} - W_{j_1} \geqq \beta_k + W_k - W_l.$$

Now by the weak reversibility assumption, $W_{j_1} \geqq W_l$, and so

$$\beta_{i_1} + W_{i_1} \geqq \beta_k + W_k;$$

that is,

$$\alpha(C_1) \geqq \alpha(C_2),$$

which is a contradiction.

If case (2) is true, then there is a path from j_1 to i_1 that does not pass through any states with costs larger than i_1. Again, identify the particular arc of that path that exits C_2 as (k, l). Note that

$$\begin{aligned}\beta_{i_1} &= \beta_{i_1,j_1} \\ &= \beta_{i_2,j_2} \\ &\geqq \beta_{kl}.\end{aligned}$$

Using similar arguments as in case (1), since $\beta_{i_1} \geqq 0$ we have $\beta_{i_1} \geqq \beta_k + W_k - W_l$. Now by the weak reversibility assumption $W_{i_1} \geqq W_l$, and so $\alpha(C_1) \geqq \alpha(C_2)$, which is again a contradiction.

Hence there is only one equipotential set, A. □

Since $W_i + \beta_i = \alpha(A)$ for all $i \in A$, where A is a recurrently connected set, we obtain the following necessary and sufficient condition for simulated annealing to hit a *global minimum* with probability one from all states $i \in X$.

Let $M := \{i \in X: W_i \leqq W_j \text{ for all } j \in X\}$ be the set of global minima. We now have the following definition due to [1].

DEFINITION 7. Let d^* be the *smallest* number with the property that for every $i \in X$ there exists a path $(i = i_0, \cdots, i_p)$ with $c_{i_k,i_{k+1}} > 0$ for $0 \leqq k \leqq p-1$ and ending in a minimizer $i_p \in M$ such that

$$W_{i_k} - W_i \leqq d^* \quad \text{for } k = 1, \cdots, p.$$

We shall call d^* the *depth* of the minimization problem.

THEOREM 6 (Necessary and Sufficient Condition to Hit Global Minimum With Probability One). *Suppose that weak reversibility holds.*

(1) *If* $\sum_{t=1}^{\infty} \epsilon(t)^{d^*} = +\infty$, *then for every initial condition* $x(0) \in X$,

$$\limsup_{N \to \infty} \frac{1}{N} \sum_{t=1}^{N} \Pr(x(t) \in M) = 1,$$

and the global minimum is hit with probability one.

(2) *If* $\sum_{t=1}^{\infty} \varepsilon(t)^{d^*} < +\infty$, *then there exists an initial condition* $x(0) \in X$ *for which*

$$\Pr(x(t) \in M^c \text{ for all } t \geqq 1) > 0.$$

Proof. The proof is the same as in Theorem (4.6) in [7] except that if $(i = i_0, \cdots, i_p = j)$ is a path from i to j with $c_{i_k, i_{k+1}} > 0$ and $W_{i_k} - W_i \leqq \gamma$ for $1 \leqq k \leqq p$, then instead of using the reversed path $(j = i_p, \cdots, i_0 = i)$ given by the assumption of symmetric neighborhoods, we use the path $(j = l_0, \cdots, l_q = i)$ with $c_{l_k, l_{k+1}} > 0$ and $W_{l_k} - W_i \leqq \gamma$ for $1 \leqq k \leqq q$, guaranteed by the weak reversibility assumption. □

The same condition $\sum_{t=1}^{\infty} \varepsilon(t)^{d^*} = \infty$ has been shown earlier by Hajek [1] to be necessary and sufficient for $\lim_{t \to \infty} \Pr(x(t) \in M) = 1$, i.e., for convergence *in probability*. Thus while result (1) above is weaker than his, since it involves Cesaro as opposed to regular convergence, the result (2) is a stronger sample path result.

The above result has been proved earlier in [7] under the stronger assumption of *symmetric neighborhoods*, $c_{ij} > 0 \Leftrightarrow c_{ji} > 0$. Moreover, under this assumption Connors and Kumar [7] have proved a *detailed balance* result that we can obtain as a corollary of Theorem 5, as we show below.

COROLLARY 1 (Detailed Balance). *Under the symmetric neighborhood assumption,*

$$\beta_{ij} = \beta_{ji} \quad \text{for every } i, j \in X.$$

Proof. If i and j are not neighbors, then $\beta_{ij} = \beta_{ji} = -\infty$.

If i and j are neighbors and $i \in R$ and $j \in T$, where R is the set of recurrent states and T is the set of transient states, then

$$\beta_{jk} = -\infty \quad \text{for all } k$$

and so

$$-\infty = \max_{k \neq j} \beta_{jk} = \max_{k \neq j} \beta_{ki} \geqq \beta_{ij},$$

showing that $\beta_{ij} = \beta_{ji} = -\infty$. A similar argument holds if $i \in T$ and $j \in R$.

Finally, if i and j are neighbors and $i, j \in R$, without loss of generality let us assume that $W_i \geqq W_j$. Then $\beta_{ij} = \beta_i \geqq 0$, and so i and j belong to a common recurrently connected set. Hence by Theorem 5, $\beta_i + W_i = \beta_j + W_j$. Since $\beta_{ij} = \beta_i$ and $\beta_{ji} = \beta_j + W_j - W_i$, it follows that $\beta_{ij} = \beta_{ji}$. □

Note that by the above results, if the order of recurrence of even *one* state in a connected component is known, then the orders of recurrence for *all* the states belonging to the connected component are determined. However, as Example 4 shows, it is not always possible to determine the order of recurrence of even one state in a connected component from the order balance equations alone. In that example, the connected components of recurrent states are the sets $\{1\}$ and $\{2\}$, and the detailed balance equations do not determine the order of recurrence β_2 of the *single* state in the connected component $\{2\}$. The reason for this inadequacy, as mentioned earlier in Example 4, is that the orders of recurrence do depend on the proportionality constants c_{ij} involved in the transition probabilities. In any case, the β-flows do satisfy Corollary 1.

6. Conclusions. The notion of order of recurrence provides a novel approach for analyzing the class of Markov chains whose transition probabilities are proportional to powers of a time-varying parameter $\varepsilon(t)$. These recurrence orders satisfy a set of balance equations, and the Markov chain converges in a Cesaro sense to the set of states with the largest recurrence orders. We have given an algorithm for generating a solution to the order balance equations and have also provided a method for characterizing all solutions to these equations. The algebraic methods presented in this

paper for solving the order balance equations are not always sufficient for determining the recurrence orders. In some situations where nonunique solutions exist, the orders of recurrence can depend on the proportionality constants involved in the transition probabilities, and not just on their orders of magnitude. This problem remains an open issue. The method of optimization by simulated annealing falls within the framework of this class of Markov chains. We have shown that if the Markov process is weakly reversible, then the sum of the recurrence order and the cost are constants on each sets of states connected by recurrent arcs. This allows us to determine the necessary and sufficient conditions on the cooling rate for the optimization algorithm to hit a global minimum with probability one from all initial states.

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SIMULATED-ANNEALING TYPE MARKOV CHAINS AND THEIR ORDER BALANCE EQUATIONS*

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Abstract

We consider generalized simulated-annealing type Markov chains where the transition probabilities are proportional to powers of a vanishing small parameter. One can associate with each state an "order of recurrence" which quantifies the asymptotic behavior of the state occupation probability. These orders of recurrence satisfy a fundamental balance equation across every edge-cut in the graph of the Markov chain. Moreover, the Markov chain converges in a Cesaro-sense to the set of states having the largest recurrence orders. We provide graph theoretic algorithms to determine the solutions of the balance equations. By applying these results to the problem of optimization by simulated annealing, we show that the sum of the recurrence order and the cost is a constant for all states in a certain connected set, whenever a "weak-reversibility" condition is satisfied.

1 Introduction

We consider finite state Markov chains $\{x(t)\}$ with transition probabilities of the type,

$$p_{ij}(t) = c_{ij}\epsilon(t)^{V_{ij}},$$

where $\epsilon(t)$ is a small parameter converging to zero. In a previous paper [1] we have shown that if one defines "orders of recurrence" by (more precise definitions are given in Section 2),

$$\beta_i := \sup\{c \geq 0 : \sum_{t=0}^{\infty} \epsilon(t)^c \pi_i(t) = +\infty\},$$

then

(i) these recurrence orders satisfy a balance equation,

$$\max_{i \in A, j \in A^c}(\beta_i - V_{ij}) = \max_{i \in A, j \in A^c}(\beta_j - V_{ji}),$$

for every subset A, and

(ii) the Markov process converges to the set of states with the largest orders of recurrence.

This provides a novel approach to analyzing the asymptotic behavior of such time-inhomogeneous Markov processes. Specifically, one uses (i) to solve the balance equations, and then (ii) provides the limiting behavior. Moreover the orders of recurrence also provide information about the rates of convergence of the state occupation probabilities. This approach via recurrence orders therefore converts the analytic problem of determining the asymptotic behavior of the time-inhomogeneous process into a purely algebraic problem of solving the balance equations.

A significant motivation for studying such Markov chains lies in the fact that in the method of optimization by simulated annealing, *if* $\{W_i\}$ *is the cost function whose minimum is sought, then one obtains* a Markov chain with,

$$p_{ij}(t) = c_{ij}\epsilon(t)^{\max(0, W_j - W_i)}.$$

Thus simulated annealing is a special case where the powers V_{ij} satisfy,

$$V_{ij} := \max(0, W_j - W_i),$$

for some $\{W_i\}$.

In order to pursue the above approach for analyzing such time-inhomogeneous Markov chains, it is necessary to be able to solve the balance equations. However, there can be non-unique solutions to the balance equations. We present graph-theoretic circulation based algorithms to obtain *a* solution, as well as *all* solutions, to the balance equations. We show by an example the interesting phenomenon that such non-uniqueness can arise when the asymptotic properties of the Markov process, and the recurrence orders, depend not just on the *exponents* V_{ij}, but also on the *proportionality constants* c_{ij}.

By applying these results to the Markov chain arising from the method of optimization by simulated annealing when the "weak reversibility" condition of Hajek [2] holds, we show that the sum of the recurrence order and the cost is a constant on sets connected by recurrent arcs. This allows us to obtain the necessary and sufficient condition for the optimization algorithm to hit the global minimum with probability one. Our necessity result is a stronger sample path result than is found in [2] or [3].

Background

Tsitsiklis [3] has also investigated Markov chains with transition probabilities proportional to powers of a small time-varying parameter. His analysis was based on observing that due to the slow variation of $\{\epsilon(t)\}$, one can employ bounds on the state occupation probabilities for *stationary* Markov chains, where $\epsilon(t)$ is held constant, to obtain bounds for the time-inhomogeneous case. His approach is quite different from ours.

Based on an analogy to the physical process of annealing, the sequence $\epsilon(t)$ is called the "cooling schedule," and just as in the physical analogy it plays a key role in determining asymptotic behavior. It was shown by Geman and Geman [4], Mitra, Romeo and Sangiovanni-Vincentelli [5], and Gidas [6], that simulated annealing converges in probability to a minimum of the optimization problem provided $\sum_{t=0}^{\infty} \epsilon(t)^p = +\infty$ for large enough p. Hajek [2] has determined the necessary and sufficient conditions on the value of p for the algorithm to converge *in probability* to the minimum when a "weak reversibility" assumption is satisfied.

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2 Orders of Recurrence and Balance Equations

Consider a Markov chain over a finite state space X whose transition probabilities are proportional to *powers* of a vanishing time varying parameter $\epsilon(t)$; that is, the transition probabilities $p_{ij}(t) := \Pr(x(t+1) = j | x(t) = i)$ are given by,

$$p_{ij}(t) = c_{ij}\epsilon(t)^{V_{ij}}, \qquad \text{for all } i,j \in X, i \neq j, \text{ and } t \in Z^+, \tag{1}$$

where

$$0 \leq V_{ij} \leq +\infty, \qquad \text{for all } i,j \in X, i \neq j, \tag{2}$$

$$c_{ij} \geq 0, \qquad \text{for all } i,j \in X, i \neq j, \text{ and } \sum_j c_{ij} = 1 \text{ for all } i. \tag{3}$$

Regarding the small parameter $\{\epsilon(t)\}$, we will assume that,

$$0 < \epsilon(t) < 1, \qquad \text{for all } t \in Z^+ \tag{4}$$

$$\exists M < \infty \text{ such that } \epsilon(t) \leq M\epsilon(s) \text{ whenever } t \geq s, \tag{5}$$

and

$$\sum_{t=1}^{\infty} \epsilon(t)^p < \infty, \qquad \text{for some } p \in [1, +\infty). \tag{6}$$

In what follows we will assume that in (1-3) we have

$$c_{ij} = 0 \Longleftrightarrow V_{ij} = +\infty$$

which is clearly without any loss of generality.

Let $\pi_i(t) := \Pr(x(t) = i)$ be the probability distribution of $x(t)$, and $\pi_{ij}(t) := \Pr(x(t) = i, x(t+1) = j)$ be the probability of a *transition* from state i to j at time t.

We define the *recurrence orders* for the states and transitions of the Markov process, as follows.

Definition 2.1 *The order of recurrence of a state $i \in X$, denoted β_i, is*

$$\beta_i := \begin{cases} -\infty & \text{if } \sum_{t=0}^{\infty} \pi_i(t) < +\infty, \\ p^- & \text{if } p = \sup\{c \geq 0 : \sum_{t=0}^{\infty} \epsilon(t)^c \pi_i(t) = +\infty\} \\ & \quad \text{and } \sum_{t=0}^{\infty} \epsilon(t)^p \pi_i(t) < +\infty, \\ p & \text{if } p = \max\{c \geq 0 : \sum_{t=0}^{\infty} \epsilon(t)^c \pi_i(t) = +\infty\}. \end{cases}$$

We say a state i is transient if $\beta_i = -\infty$; otherwise we say the state is recurrent.

In a similar manner we define the *order of recurrence of the transition from i to j*, β_{ij}, by replacing $\pi_i(t)$ with $\pi_{ij}(t)$ in the definition above. Again, we say the transition from i to j is *transient* if $\beta_{ij} = -\infty$; otherwise we say the transition is *recurrent*.

It is also convenient to define ρ, the *order of cooling* of $\{\epsilon(t)\}$, as follows.

Definition 2.2 *The order of the cooling schedule $\{\epsilon(t)\}$, denoted ρ, is defined as,*

$$\rho := \begin{cases} -\infty & \text{if } \sum_{t=0}^{\infty} \epsilon(t) < +\infty, \\ p^- & \text{if } p = \sup\{c \geq 0 : \sum_{t=0}^{\infty} \epsilon(t)^c = +\infty\} \\ & \quad \text{and } \sum_{t=0}^{\infty} \epsilon(t)^p < +\infty, \\ p & \text{if } p = \max\{c \geq 0 : \sum_{t=0}^{\infty} \epsilon(t)^c = +\infty\}. \end{cases}$$

The relationship between β_i, β_{ij} and ρ is given in the following Lemma 2.1. It will be convenient in the sequel to define the operation "$\ominus$" as follows:

$$a \ominus b := \begin{cases} -\infty & \text{if } a < b \\ a - b & \text{if } a \geq b. \end{cases}$$

Lemma 2.1 *β_{ij} and β_i are related by*

$$\beta_{ij} = \beta_i \ominus V_{ij}, \qquad \text{for all } i,j \in X, \tag{7}$$

and ρ and β_i are related by,

$$\max_{i \in X} \beta_i = \rho. \tag{8}$$

Proof: See [1]. ∎

Knowledge of the β_i's provides useful information about the asymptotic properties of $\{x(t)\}$. The following theorem shows that the time-inhomogeneous Markov chain converges in a *Cesaro sense* to the set of states having the largest orders of recurrence.

Theorem 2.1 *Let $\mathcal{M}$ be the set of states with the largest orders of recurrence,*

$$\mathcal{M} := \{i \in X : \beta_i = \rho\}.$$

Then

$$\limsup_{N \to \infty} \frac{1}{N} \sum_{t=1}^{N} \Pr(x(t) \in \mathcal{M}) = 1. \tag{9}$$

Proof: See [7]. ∎

Our goal therefore is to determine the recurrence orders, and critical to that will be the following result established in [1], which shows that there is a fundamental balance of recurrence orders across every edge-cut in the graph of the Markov chain.

Theorem 2.2 (Order Balance)

$$\max_{i \in A, j \in A^c} \beta_{ij} = \max_{i \in A, j \in A^c} \beta_{ji}, \qquad \text{for every } A \subseteq X. \tag{10}$$

Equivalently, using the "$\ominus$" notation and (7),

$$\max_{i \in A, j \in A^c} \beta_i \ominus V_{ij} = \max_{i \in A, j \in A^c} \beta_j \ominus V_{ji}, \qquad \text{for every } A \subseteq X. \tag{11}$$

Proof: See [1]. ∎

Note that through Theorems 2.1 and 2.2 we have converted the *problem* of determining the asymptotic properties of the time-inhomogeneous Markov chain into an *algebraic* problem of solving the balance equations (10).

3 The Modified Balance Equations

Note that if $(\beta_1, \beta_2, \ldots, \beta_{|X|})$ satisfy (11), then $(\beta_1 - a, \beta_2 - a, \ldots, \beta_{|X|} - a)$ also satisfy (11) for every a, i.e. the solution set is *translation invariant*. Thus the equation (8) which fixes the maximum of the β_i's needs to also be taken into account.

However, (11, 8) can together *still* possess non-unique solutions for sufficiently small values of ρ. In this section, we will show how one can obtain *one* solution to (11, 8); in the next section we show how to obtain *all* solutions.

It is convenient to consider the following "modified" balance equations, which as we show in the sequel, always possess a unique solution. Given $\rho \geq 0$ and $V_{ij} \geq 0$ for $i,j = 1, \ldots, |X|$ with $i \neq j$, consider the problem of determining $\lambda := (\lambda_1, \ldots, \lambda_{|X|})$ such that

$$\max_{i \in A, j \in A^c} \lambda_i - V_{ij} = \max_{i \in A, j \in A^c} \lambda_j - V_{ji}, \qquad \text{for every } A \subsetneq \{1, \ldots, |X|\}, \tag{12}$$

and

$$\max_i \lambda_i = \rho. \tag{13}$$

We call (12, 13) the "modified" balance equations. Observe that (12) differs from (11) in that the operation "$-$" is used in place of "$\ominus$." Also, the λ's can be negative in (12).

We have introduced the modified balance equations in order to avoid the difficulties in handling $-\infty$ that occur under the "$\ominus$" operation. The following theorem gives properties of solutions to the order balance and modified balance equations

Theorem 3.1 *1. If λ satisfies the modified balance equations for a given ρ and V, then β defined by,*

$$\beta_i := \lambda_i \ominus 0 \tag{14}$$

satisfies the order balance equations (11, 8) for the given ρ and V.

2. *For every given ρ and V, there exists a unique solution λ to the modified balance equations. Moreover, the solutions for different values of ρ are translates of each other.*

3. *Whenever ρ is large enough, there exists a unique solution to the order balance equations (11, 8). These unique solutions are all translates of the solutions for the modified balance equations.*

Proof: See [7]. ■

We now give an algorithm for determining the *unique* solution to the modified balance equations. An illustrative example is convenient.

Example 3.1 Let $\rho = 5$ and

$$V = [V_{ij}] = \begin{pmatrix} \star & 4 & 3 & 1 \\ 6 & \star & 3 & 7 \\ 6 & 2 & \star & 4 \\ 2 & 6 & 5 & \star \end{pmatrix}.$$

Our goal is to determine $\lambda = (\lambda_1, \ldots, \lambda_4)$ which satisfies (12, 13). We shall refer to $\lambda_i - V_{ij}$ as the *λ-flow* along the arc (i,j). Consider first the modified balance equation for the edge cut $A = \{i\}$,

$$\max_{j \neq i} \lambda_i - V_{ij} = \max_{j \neq i} \lambda_j - V_{ji}. \tag{15}$$

Observe that the LHS of (15) can be written as

$$\lambda_i - \min_{j \neq i} V_{ij},$$

and so the arc of *maximum λ-flow* out of $A = \{i\}$ is the arc $(i, l(i))$ where

$$l(i) = \arg\min_{j \neq i} V_{ij}.$$

(Note that $l(i)$ may not be unique.)

We now construct the directed graph $G_1 = (V_1, E_1)$, with $V_1 = \{\{1\}, \ldots, \{4\}\}$ and $(i,j) \in E_1$ if $j = l(i)$. Note that G_1 has two directed cycles $\{1\} \longrightarrow \{4\} \longrightarrow \{1\}$ and $\{2\} \longrightarrow \{3\} \longrightarrow \{2\}$. Let us examine the λ-flows on the directed cycle $\{1\} \longrightarrow \{4\} \longrightarrow \{1\}$. Since $\lambda_1 - V_{14}$ is the maximum λ-flow out of $\{1\}$, it is not smaller than any λ-flow into $\{1\}$, and so in particular

$$\lambda_1 - V_{14} \geq \lambda_4 - V_{41}.$$

Also, $\lambda_4 - V_{41}$ is the maximum λ-flow out of $\{4\}$ and so

$$\lambda_4 - V_{41} \geq \lambda_1 - V_{14}.$$

We thus observe that the λ-flows along the directed cycle $\{1\} \longrightarrow \{4\} \longrightarrow \{1\}$ are equal; that is,

$$\lambda_1 - V_{14} = \lambda_4 - V_{41},$$

and so

$$\lambda_1 - 1 = \lambda_4 - 2. \tag{16}$$

Thus, we have determined the *difference* between λ_1 and λ_4.

In exactly the same way, from the directed cycle $\{2\} \longrightarrow \{3\} \longrightarrow \{2\}$ we see that

$$\lambda_2 - 3 = \lambda_3 - 2. \tag{17}$$

thus determining the difference between λ_2 and λ_3.

At the next step of the algorithm, consider the modified balance equations for the edge cut (A, A^c) where $A = \{1,4\}$ and $A^c = \{2,3\}$. Observe that for $A = \{1,4\}$, the LHS of the modified balance equation

$$\max_{i \in A, j \in A^c} \lambda_i - V_{ij} = \max_{i \in A, j \in A^c} \lambda_j - V_{ji} \tag{18}$$

can be written as

$$\max(\lambda_1 - V_{12}, \lambda_1 - V_{13}, \lambda_4 - V_{42}, \lambda_4 - V_{43});$$

that is,

$$\max(\lambda_1 - 4, \lambda_1 - 3, \lambda_4 - 6, \lambda_4 - 5).$$

We have previously determined that $\lambda_4 - \lambda_1 = 1$, and so the maximum is achieved by $\lambda_1 - V_{13} = \lambda_4 - 3$, and the arc of maximum λ-flow out of $\{1,4\}$ is the arc $(1,3)$.

In a similar fashion, examining the RHS of the modified balance Equation (18), we determine that the maximum λ-flow out of $\{2,3\}$ is achieved by $\lambda_3 - V_{34} = \lambda_3 - 4$, and so the arc of maximum λ-flow out of $\{2,3\}$ is the arc $(3,4)$.

We now consider the directed graph $G_2 = (V_2, E_2)$, with $V_2 = \{\{1,4\}, \{2,3\}\}$ and $E_2 = \{(1,3), (3,4)\}$. Note that E_2 is the set of the arcs of maximum λ-flow out of the edge cuts in V_2.

Observe that G_2 has a directed cycle $\{1,4\} \longrightarrow \{2,3\} \longrightarrow \{1,4\}$. Now note that $\lambda_1 - V_{13}$ is the maximum λ-flow out of $\{1,4\}$ and $\lambda_3 - V_{34}$ is the maximum λ-flow out of $\{2,3\}$ and so

$$\lambda_1 - V_{13} = \lambda_3 - V_{34};$$

that is,

$$\lambda_1 - 3 = \lambda_3 - 4. \tag{19}$$

Combining (16, 17, 19) gives

$$\lambda_1 - 3 = \lambda_2 - 5 = \lambda_3 - 4 = \lambda_4 - 4. \tag{20}$$

We now know the *pairwise differences* between *all* of the λ_i's, and so we do not need to consider any additional edge cuts. To fix the values of $\{\lambda_i\}$, we use the value of ρ to give,

$$\max_{i \in X} \lambda_i = \rho = 5$$

Since, from (20), λ_2 is the largest, we set $\lambda_2 = 5$. We thus obtain the solution to the modified balance equations as,

$$\lambda_1 = 3, \qquad \lambda_2 = 5, \qquad \lambda_3 = \lambda_4 = 4.$$

■

The principal idea used to solve the modified balance equations in Example 3.1 is summarised in the following lemma.

Lemma 3.1

1. *Given $A \subseteq X$ for which we know the pairwise differences between all the λ_i's for states in A, we can determine the arc of maximum λ-flow out of A (without knowing the λ_i's themselves).*

2. *Let $A_1, A_2, \ldots, A_p$ be a partition of X and suppose for each A_k we know all the pairwise differences between the λ_i's for all states in A_k. Let (i_k, j_k) denote the arc of maximum λ-flow out of A_k. Construct the directed graph $G = (V, E)$, with $V = \{A_1, \ldots, A_p\}$ and $E = \{(i_1, j_1), \ldots, (i_p, j_p)\}$. There exists a directed cycle on G. If $\{A_{m_1}, \ldots, A_{m_m}\}$ is the list of vertices, in order, along the directed cycle, then the λ-flow on the directed cycle is constant; that is,*

$$\lambda_{i_{m_1}} - V_{i_{m_1} j_{m_1}} = \cdots = \lambda_{i_{m_m}} - V_{i_{m_m} j_{m_m}},$$

and we can determine the pairwise differences between the values of the λ_i's for all the states in $\bigcup_{k=1}^{p} A_k$.

Proof: See [7]. ■

The algorithm for solving the modified balance equations is outlined below.

Algorithm to solve modified balance equations

Step 1: Set $A_i^1 = \{i\}$ for $i = 1, \ldots, |X|$. We call the A_i^k's *coalitions at step k*. Note that for every i, the pairwise differences between the λ-values for all states in A_i^1 are (trivially) known. Set $A^1 := \{A_1^1, A_2^1, \ldots, A_{|X|}^1\}$. Let $N(1) = |A^1| =:$ the number of elements in the set A^1 = number of coalitions at Step 1.

Step k: Given $A^k := \{A_1^k, A_2^k, \ldots, A_{N(k)}^k\}$, where for each $A_j^k \in A^k$ the pairwise differences between all of the λ_i's for i's in A_j^k are known, construct A^{k+1} as follows. Using Lemma 3.1, identify the directed cycles in the graph. (There exists at least one directed cycle.) The elements of A^{k+1} consist of the directed cycles

identified in the graph, and those $A_j^k \in A^k$ which are not in any directed cycle. (More precisely, if $\{A_{i_1}^k, A_{i_2}^k, \ldots, A_{i_m}^k\}$ is a directed cycle, then $\bigcup_{l=1}^m A_{i_l}$ is an element of A^{k+1}). Note that for every $A_j^{k+1} \in A^{k+1}$, the pairwise differences between all of the λ_i's for i's in A_j^{k+1} are known. Furthermore, if $N(k) := |A^k|$, then $N(k+1) < N(k)$.

st Step: Stop when $N(k) = 1$. Note that the pairwise differences between *all* λ_i's are known, and the λ satisfying the modified balance equations can be obtained by a translation by using the given value of ρ. ■

An Algorithm to Obtain All Solutions of the Order Balance Equations

e now characterize *all* solutions to the order balance equations, d describe an algorithm for generating *all* these solutions. To do we will use the coalitions $\{A_i^k\}$ generated by the algorithm of the eceding section. Let us call $\lambda_i - V_{ij}$ and $\beta_{ij} = \beta_i \ominus V_{ij}$ as the *λ-flow* d *β-flow*, respectively, along the arc (i,j).

mma 4.1 *1. If (i,j) is the arc of maximum λ-flow out of A_l^k, then it is also the arc of maximum β-flow out A_l^k.*

2. If $\{A_{i_1}^k, \ldots, A_{i_p}^k\}$ is a directed cycle obtained at step k, then the β-flow along the directed cycle is a constant.

3. If the β-flow along the directed cycle $\{A_{i_1}^k, \ldots, A_{i_p}^k\}$ obtained at step k is $-\infty$, then the β-flow along any directed cycle obtained at step $n > k$ containing $A_l^n = \bigcup_{m=1}^p A_{i_m}^k$ as a node, is also $-\infty$.

4. If the β-flow along the directed cycle $\{A_{i_1}^k, \ldots, A_{i_p}^k\}$ obtained at step k is ≥ 0, then for every $i,j \in A_l^{k+1} := \bigcup_{m=1}^p A_{i_m}^k$ there exists a path $(i = i_0, i_1, \ldots, i_q = j)$ such that $i_m \in A_{l_m}^{k+1}$ and $\beta_{i_m,i_{m+1}} \geq 0$ for $0 \leq m \leq q-1$.

roof: See [7]. ■

Motivated by 3) and 4) above, we introduce the following defini-n.

efinition 4.1 *We shall say that i is* recurrently connected *to j there exists a path $(i = i_0, i_1, \ldots, i_q = j)$ with $\beta_{i_m,i_{m+1}} \geq 0$ for $\leq m \leq q-1$.*

We shall say that a set $A \subseteq X$ is a recurrently connected set *if r every $i,j \in A$ and $k \in A^c$, i is recurrently connected to j but not k.*

From Lemma 4.1 it follows that recurrently connected sets are ecisely those A_l^k's for which the β-flow out of A_l^k is $-\infty$, while the flows along the directed cycles contained within A_l^k are ≥ 0. Note o that the recurrently connected *sets* form a *partition of X*.

We now proceed to determine which sets are possible candidates being recurrently connected sets. Consider a typical candidate $^{+1}$. Let $\mathcal{F}$ denote the β-flow on the cycle $\{A_{i_1}^k, \ldots, A_{i_p}^k\}$, where $^{+1} = \bigcup_{l=1}^p A_{i_l}^k$. Then if (i_m, j_m) is the arc of maximum flow out of , (and, by construction, into $A_{(m+1) \bmod p}^k$), we must have,

$$\mathcal{F} = \beta_{i_1} - V_{i_1,j_1} = \beta_{i_2} - V_{i_2,j_2} = \cdots = \beta_{i_p} - V_{i_p,j_p} \geq 0,$$

$$\max_{i \in A_l^{k+1}, j \notin A_l^{k+1}} \beta_i - V_{ij} < 0,$$

d

$$\max_{i \in A_l^{k+1}} \beta_i \leq \rho.$$

e will now attempt to determine whether there exist $\{\beta_i : i \in A_l^{k+1}\}$ hich satisfy these conditions. Note that if this is not feasible, then $^{+1}$ cannot be a recurrently connected set.

Let (x,y) denote the arc of maximum β-flow out of A_l^{k+1}. Then $< V_{xy}$. Fix m to be an arbitrarily chosen state from A_l^{k+1}. Then for every state $h \in A_l^{k+1}$ we know the value of $(\beta_h - \beta_m)$ from Lemma 4.1 above. Let us define

$$\zeta_h := \beta_h - \beta_m.$$

Then

$$\begin{aligned} \mathcal{F} &= \beta_{i_1} - V_{i_1,j_1} \\ &= \beta_m + \zeta_{i_1} - V_{i_1,j_1} \\ &= \beta_x - \zeta_x + \zeta_{i_1} - V_{i_1,j_1} \\ &< V_{xy} - \zeta_x + \zeta_{i_1} - V_{i_1,j_1} =: M_1, \end{aligned}$$

giving an upper bound on $\mathcal{F}$.

We must also satisfy the constraint $\max_{i \in A_l^{k+1}} \beta_i \leq \rho$, and so let

$$\theta := \arg \max_{i \in A_l^{k+1}} \zeta_i.$$

Then it is clear that $\beta_\theta \geq \max_{i \in A_l^{k+1}} \beta_i$. Thus,

$$\begin{aligned} \rho &\geq \beta_\theta \\ &= \beta_m + \zeta_\theta \\ &= \beta_{i_1} - \zeta_{i_1} + \zeta_\theta \\ &= \beta_{i_1} - V_{i_1,j_1} + V_{i_1,j_1} - \zeta_{i_1} + \zeta_\theta \\ &= \mathcal{F} + V_{i_1,j_1} - \zeta_{i_1} + \zeta_\theta, \end{aligned}$$

and so

$$\mathcal{F} \leq \rho - V_{i_1,j_1} + \zeta_{i_1} - \zeta_\theta =: M_2.$$

giving yet another upper bound on $\mathcal{F}$. (Note: if $A_l^{k+1} = \{i\}$, then $M_1 = \min_j V_{ij}$ and $M_2 = \rho$.)

Any choice of $\mathcal{F}$ from the interval

$$\Omega(A_l^{k+1}) := [0, M_1) \bigcap [0, M_2]$$

will allow assignments for the recurrence orders of states in A_l^{k+1} consistent with the assumption that the coalition A_l^{k+1} is a recurrently connected set. If $\Omega(A_l^{k+1}) = \phi$ then there is no assignment, and so A_l^{k+1} is not a recurrently connected set.

We still need to determine the set of all recurrently connected sets. To do this we construct a *rooted tree* having the coalitions produced by the general procedure as nodes, and having a directed edge from coalition A_p^{k+1} to A_r^k if $A_p^{k+1} \supseteq A_r^{(k)}$. Hence, the root of the tree is X, and its leaves are the singleton sets $\{1\}, \{2\}, \ldots, \{n\}$. Let D_i be the set of the leaves of the tree which are *descendants* of the node i in the rooted tree.

We say that a set Ξ of nodes is a *proper cover* if

$$\bigcup_{A \in \Xi} D_A = X$$

and

$$D_A \bigcap D_{A'} = \phi \qquad \text{for } A \neq A'.$$

Now the algorithm to determine all the solutions of (11,8) proceeds as follows. Let a set $\Xi := \{A_1, A_2, \ldots, A_k\}$ be a proper cover. Now we will determine whether Ξ can be a set of *all* recurrently connected sets, as follows. First we determine $\Omega(A_j)$ for every $A_j \in \Xi$. If *any* of the $\Omega(A_j)$'s is empty, then the guess Ξ is *not* a feasible set of recurrently connected sets. If every $\Omega(A_j)$ is non-empty, then let $\overline{\mathcal{F}}_j := \max \Omega(A_j)$, and for each A_j determine whether with the choice of $\overline{\mathcal{F}}_j$ there is a state $i_j \in A_j$ with $\beta_{i_j} = \rho$. If no such state exists for *any* A_j, then again Ξ is *not* a feasible set of recurrently connected sets. Finally, if there exist such A_j's, then let $\mathcal{A}(\Xi)$ be the set of all such A_j's. Now, the set of all solutions corresponding to Ξ is obtained by picking, in turn, an A_j from $\mathcal{A}(\Xi)$, fixing its flow as $\overline{\mathcal{F}}$, and choosing all other $\mathcal{F}_j$'s arbitrarily from the $\Omega(A_j)$'s. By checking every proper cover Ξ, we thus determine all solutions to the order balance equations. See [7] for the precise proof.

We illustrate the procedure for determining all solutions to the order balance equations.

Example 4.1 We construct all solutions to the order balance equations for Example 3.1 when $\rho = 4$. We check the proper covers:

1. $\Xi = \{X\}$: $\Omega(\{1,4\})$ is empty, so X cannot be a recurrently connected set.
2. $\Xi = \{\{1,4\},\{2,3\}\}$: Using the method described above we obtain
$$\beta_1 = \alpha, \quad \beta_2 = 4, \quad \beta_3 = 3, \quad \beta_4 = 1 + \alpha,$$
where $1 \le \alpha < 3$.
3. $\Xi = \{\{1,4\},\{2\},\{3\}\}$: $\max_{i \in X} \beta_i < 4$, a contradiction.
4. $\Xi = \{\{1\},\{4\},\{2,3\}\}$:
$$\beta_1 = \gamma, \quad \beta_2 = 4, \quad \beta_3 = 3, \quad \beta_4 = \theta,$$
where $\gamma = -\infty$ or $0 \le \gamma < 1$, and $\theta = -\infty$ or $0 \le \theta < 2$.
5. $\Xi = \{\{1\},\{2\},\{3\},\{4\}\}$: $\max_{i \in X} \beta_i < 4$, and so $\{\{1,4\},\{2,3\}\}$ is not a set of recurrently connected sets.

We have checked all proper covers. Hence the set of all solutions is $\{(\alpha, 4, 3, 1+\alpha) : 1 \le \alpha < 3\} \cup \{(\gamma, 4, 3, \theta) : \gamma = -\infty$ or $0 \le \gamma < 1$ and $\theta = -\infty$ or $0 \le \theta < 2\}$. ■

How can non-unique solutions to the order balance equations arise, and what is the implication of such non-uniqueness? First let us consider the case where a unique solution exists. Since such a solution is uniquely determined by the algorithm, it is clear that the recurrence orders of the states, and thus the rates of convergence of the transition probabilities, depend only on the V_{ij}'s in the transition probabilities $p_{ij}(t) = c_{ij}c(t)^{V_{ij}}$, and not on the proportionality constants $\{c_{ij}\}$. However, in the case of non-unique solutions, the following example shows that the recurrence orders may even depend on the the *proportionality constants* $\{c_{ij}\}$.

Example 4.2 Let $X = \{1,2,3\}$ and $V_{ij} = \max\{0, j-i\}$. Let $c_{13} = c_{23} = 1$, $c_{31} = 1-\alpha$ and $c_{32} = \alpha$, where $\alpha \in (0,1)$. Set $c_{ij} = 0$ for all other i,j. Let the cooling schedule be $c(t) = 1/t$. Then the *complete* set of order balance equations obtained by using *all* edge cuts is,

$$\begin{aligned} \beta_2 \ominus V_{23} &= \beta_3 \ominus V_{33}, \\ \beta_3 \ominus V_{31} &= \beta_1 \ominus V_{13}, \\ \max(\beta_2 \ominus V_{23}, \beta_1 \ominus V_{13}) &= \max(\beta_3 \ominus V_{33}, \beta_3 \ominus V_{31}), \end{aligned}$$

with the maximum given by,

$$\max_{i \in X} \beta_i = 1.$$

The assignments

$$\beta_1 = 1, \quad \beta_2 = \gamma, \quad \beta_3 = -\infty$$

satisfy the order balance equations for every $\gamma \in (-\infty) \cup [0,1)$. Thus any value of $\beta_2 < 1$ gives a solution of the order balance equations.

However, a calculation, which can be found in [7], shows that the correct order of recurrence of state 2 is

$$\beta_2 = \alpha.$$

Thus, the order of recurrence, and the rate of convergence of the probability $\Pr(x(t) = 2)$ to 0, depends on the proportionality constant $c_{32} = \alpha$ involved. ■

Based on the above results, we obtain the following property of the orders of recurrence of the states in a recurrently connected set.

Lemma 4.2 *Consider a recurrently connected set A.*

1. *If $\beta_i \in \mathcal{R}$ for some $i \in A$, then $\beta_j \in \mathcal{R}$ for all $j \in A$.*
2. *If for some $i \in A$, $\beta_i = p_i^-$ for some $p_i \in \mathcal{R}$, then for every $j \in A$, $\beta_j = p_j^-$ for some $p_j \in \mathcal{R}$.*

Proof: This follows immediately from the proof of Lemma 4.1. ■

Thus all recurrence orders in a recurrently connected set are of the same type, i.e. either they are all real numbers p_i, or they are all of the type p_i^-, or they are all $-\infty$ (see Definition 2.1).

This gives us the following Lemma which completes the proof of Theorem 2.1.

Lemma 4.3 *Suppose the rate of cooling is $\rho = p \in \mathcal{R}$, with $p > 0$, i.e. the maximum is achieved in Definition 2.2. If there is a state $i \in X$ for which $\beta_i = p^-$, then $\lim_{t \to \infty} \Pr(x(t) = i) = 0$.*

Proof: Suppose A is the recurrently connected class to which i belongs. Since all arcs *between* recurrently connected sets are transient, it follows from the Borel-Cantelli Lemma that along almost every sample path ω there can only be a *finite* number of transitions between different recurrently connected sets. Hence for almost every ω, $\{x(t,\omega)\}$ converges to some recurrently connected set. Hence the limit $\lim_{t \to \infty} \Pr(x(t) \in A)$ exists. Now we show that this limit is 0. Suppose not, i.e. suppose $\lim_{t \to \infty} \sum_{j \in A} \pi_j(t) = \delta > 0$. Then it follows that $\sum_{t=0}^{\infty} c(t)^p \sum_{j \in A} \pi_j(t) = +\infty$. Hence for some $j \in A$, $\beta_j = p$. But then by Lemma 4.2, $\beta_i \in \mathcal{R}$, which gives a contradiction, thus proving the lemma. ■

5 Weak Reversibility and Simulated Annealing

We now turn our attention to the special class of Markov chains arising from the method of *optimization by simulated annealing*. Recall that the Markov chains in this class satisfy (1-6) with the special choice of

$$V_{ij} := \max\{0, W_j - W_i\}.$$

In [1] it was shown that under the "symmetric neighborhood" assumption, $c_{ij} > 0$ if and only if $c_{ji} > 0$, the orders of recurrence satisfy the following *detailed order balance*,

$$\beta_{ij} = \beta_{ji} \qquad \text{for every } i,j \in X.$$

It is easy to see that the detailed order balance above is equivalent to the sum of the order of recurrence of a state and its cost being constant on recurrently connected sets.

In this section we will show that this constancy property of the sum of the recurrence order and cost on recurently connected sets continues to hold under the much weaker assumption of "weak reversibility" introduced by Hajek in [2].

Definition 5.1 *A state i is said to be reachable from state j if there is a sequence of states $j = i_0, i_1, \ldots, i_p = i$ such that $c_{i_k, i_{k+1}} > 0$ for $0 \le k \le p-1$.*

Definition 5.2 *A state i is reachable at height H from j if there is a path from j to i as in* Definition 5.1 *for which $W_{i_k} \le H$ for $0 \le k \le p$.*

Assumption 5.1 (Weak Reversibility) *For any real number H and any two states i and j, i is reachable at height H from j if and only if j is reachable at height H from i.*

In what follows we assume weak reversibility.

Theorem 5.1 (The Potential Theorem) *Under* Assumption 5.1, *for every recurrently connected set A there exists a constant $\alpha(A)$ such that $\beta_i + W_i = \alpha(A)$ for every $i \in A$.*

Proof: See [7]. ■

Since $W_i + \beta_i = \alpha(A)$ for all $i \in A$, where A is a recurrently connected set, we obtain the following necessary and sufficient condition for simulated annealing to hit a *global minimum* with probability one from all states $i \in X$.

Let $M := \{i \in X : W_i \leq W_j \text{ for all } j \in X\}$ be the set of global minima. We now have the following definition due to [2].

Definition 5.3 *Let d^* be the smallest number with the property that for every $i \in X$ there exists a path $(i = i_0, \ldots, i_p)$ with $c_{i_k i_{k+1}} > 0$ for $0 \leq k \leq p$ and ending in a minimizer $i_p \in M$ such that*

$$W_{i_k} - W_i \leq d^* \text{ for } k = 1, \ldots, p.$$

We shall call d^* the depth of the minimization problem.

Theorem 5.2 *Suppose that weak reversibility holds.*

1. *If $\sum_{t=1}^{\infty} \epsilon(t)^{d^*} = +\infty$, then for every initial condition $x(0) \in X$,*

$$\limsup_{N \to \infty} \frac{1}{N} \sum_{t=1}^{N} \Pr(x(t) \in M) = 1,$$

and the global minimum is hit with probability one.

2. *If $\sum_{t=1}^{\infty} \epsilon(t)^{d^*} < +\infty$, then there exists an initial condition $x(0) \in X$ for which,*

$$\Pr(x(t) \in M^c \text{ for all } t \geq 1) > 0.$$

Proof: The proof is the same as in Theorem (4.6) in [1] except that if $(i = i_0, \ldots, i_p = j)$ is a path from i to j with $c_{i_k i_{k+1}} > 0$ and $W_{i_k} - W_i \leq \gamma$ for $1 \leq k \leq p$, then instead of using the reversed path $(j = i_p, \ldots, i_0 = i)$ given by the assumption of symmetric neighborhoods, one uses the path $(j = l_0, \ldots, l_q = i)$ with $c_{l_k l_{k+1}} > 0$ and $W_{l_k} - W_i \leq \gamma$ for $1 \leq k \leq q$, guaranteed by the weak reversibility assumption. ■

The same condition $\sum_{t=1}^{\infty} \epsilon(t)^{d^*} = \infty$ has been earlier shown by Hajek [2] to be necessary and sufficient for $\lim_{t \to \infty} \Pr(x(t) \in M) = 1$, i.e. for convergence *in probability*. Thus while result 1) above is weaker than his since it involves Cesaro as opposed to regular convergence, the result 2) is a stronger sample path result.

It is also worth noting that if one additionally assumes the property of *symmetric neighborhoods*, $c_{ij} > 0 \iff c_{ji} > 0$, then the *detailed balance* result of [1] follows as a corollary of Theorem 5.1, as we show below.

Corollary 5.1 (Detailed Balance) *Under the symmetric neighborhood assumption,*

$$\beta_{ij} = \beta_{ji} \text{ for every } i, j \in X.$$

Proof: See [7]. ■

Note that by the above results, if the order of recurrence of even one state in a connected component is known, then the orders of recurrence for *all* the states belonging to the connected component are determined. However, as Example 4.2 shows, it is not always possible to determine the order of recurrence of even one state in a connected component. In that example, the connected components of recurrent states are the sets $\{1\}$ and $\{2\}$. We do not know the order of recurrence of the *single* state in the connected component $\{2\}$, without taking into account the proportionality constants involved in the transition probabilities. Thus, for this example the detailed balance equations are not sufficient for determining β_2. However, note that the β-flows do satisfy Corollary 5.1.

6 Conclusions

The notion of order of recurrence provides a novel approach for analyzing the class of Markov chains whose transition probabilities are proportional to powers of a time-varying parameter $\epsilon(t)$. These recurrence orders satisfy a set of balance equations, and the Markov chain converges in a Cesaro sense to the set of states with the largest recurrence orders. We have given an algorithm for generating a solution to the order balance equations and have also provided a method for characterizing all solutions to these equations. In some situations where non-unique solutions exist, the orders of recurrence can depend on the proportionality constants involved in the transition probabilities, and not just on their orders of magnitude. This problem remains an open issue.

The method of optimization by simulated annealing falls within the framework of this class of Markov chains. We have shown that if the Markov process is weakly reversible, then the sum of the recurrence order and the cost is a constant on each set of states connected by recurrent arcs. This allows us to determine the necessary and sufficient on the cooling rate for the optimization algorithm to hit a global minimum with probability one from all initial states.

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SIMULATED ANNEALING AND BALANCE OF RECURRENCE ORDERS

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ABSTRACT

Several important problems in diverse application areas such as image restoration, code design, and VLSI design, contain at their core an optimization problem whose solution crucially determines the performance of the resulting engineering system. Standard descent algorithms for such optimization problems, however, typically get trapped in local minima, and fail to reach solutions at or near the global minimum. Motivated by the problems of determining the global minima of optimization problems, the algorithm of simulated annealing for optimization has been proposed. Here we present recent results on the performance of this algorithm in reaching the global minimum of combinatorial optimization problems.

1. INTRODUCTION

Several important application areas as diverse as image restoration,[1] code design,[2] and VLSI design,[3] require at their core the solution of an optimization problem, typically combinatorial optimization problems. It is for this reason that the subject of combinatorial optimization has attracted much attention, e.g.,[4] in recent years.

However, such combinatorial optimization problems possess a large number of local minima, and standard descent schemes for solving them typically get stuck in such local minima, and fail to reach solutions at or near the global minimum. A good illustration of this fact can be found in[5] for the well-known traveling salesman problem, and this is one of the prime reasons why such problems are intrinsically hard. Indeed for the traveling salesman problem, which is one of the most well known examples of "intractable" problems, no non-trivial choice of neighborhood structure can eliminate the possibility of existence of local minima.

Motivated by the critical need to solve such problems, the algorithm for *optimization by simulated annealing* was proposed in[6]. It is inspired by the problem of growing crystals in statistical mechanics, where "annealing" is the process by which a solid is initially heated to a high temperature, and then cooled so slowly that it settles into a crystalline state corresponding to a global minimum of the energy state. The cooling needs to be slow, since too rapid a cooling schedule traps the solid in higher energy local minima which can correspond to defects in the crystalline structure.

By an analogy with the physical process of cooling which can attain states near the global minima, see also,[7] the simulated annealing procedure for optimization is a Monte-Carlo algorithm which is a slight, but important, modification of descent algorithms. It occasionally, and randomly, accepts uphill moves, in addition to always accepting downhill moves. The parameter governing the acceptance of uphill moves, is analogous to the "temperature" and it is gradually reduced to zero. The object of such a scheme is that at high "temperature" the algorithm will escape local minima, and then slowly evolve into a pure descent scheme which seeks out a global minimum.

Being inspired by statistical physics, motivated by the solution of engineering problems, and posing several mathematical questions, this algorithm has attracted the attention of physicists, engineers and mathematicians alike.

In the rest of this paper we will present some key results that have been obtained on the performance of this algorithm, as well as, an open issue on which more research is needed.

2. THE SIMULATED ANNEALING ALGORITHM

Let X be a finite set, and let W: X→R be a given cost function on X. The goal is to minimize W(x) over x ∈ X.

Corresponding to each state i ∈ X, let $N_i \subset X$ be a deleted neighborhood of X, with $i \notin X$. Let $\{q_{ij}: i \in X, j \in N_i\}$ be such that $q_{ij} \geq 0$ and $\sum_{j \in N_i} q_{ij} = 1$. Finally, let $0 < \varepsilon(t) < 1$ be a cooling schedule with $\lim_{t \to \infty} \varepsilon(t) = 0$. For simplicity, one may also assume that $\{\varepsilon(t)\}$ is monotone decreasing.

Consider the Markov chain $\{x(t)\}$ on X with transition probabilities defined by

$$p_{ij}(t) = q_{ij}\,\varepsilon(t)^{[W_j - W_i]^+} \quad \text{for } j \in N_i$$

$$= 1 - \sum_{k \in N_i} p_{ik}(t) \quad \text{for } j = i.$$

The simulated annealing procedure consists of moving through the state space X according to this Markov chain.

Essentially, the scheme consists of two steps at each iteration. Suppose that at an iteration t, x(t) = i. Then one chooses a neighbor j randomly from N_i according to the probabilities q_{ij}. If $W_j \leq W_i$, then j is accepted and x(t+1) is set to j. Thus downhill moves are readily accepted. On the other hand, if $W_j > W_i$, then j is accepted with probability $\varepsilon(t)^{W_j - W_i}$ and rejected with probability $1 - \varepsilon(t)^{W_j - W_i}$. If j is accepted then x(t+1) is set to j; otherwise if j is rejected then x(t+1) remains at i.

Thus the scheme is seen to be a simple modification of standard descent algorithms. The parameter $\varepsilon(t)$ is the analog of temperature.

In an application such as the traveling salesman problem, X will denote the set of all tours. A neighborhood structure can be imposed by deleting two arcs in the tour and replacing them with two other arcs; see[5] for examples.

3. SIMULATED ANNEALING TYPE MARKOV CHAINS

More generally, simulated annealing gives rise to a time inhomogeneous Markov chain over a finite state space X with transition probabilities given by:

$$p_{ij}(t) = q_{ij}\,\varepsilon(t)^{V_{ij}} \quad \text{if } j \in N_i$$

$$= 1 - \sum_{k \in N_i} p_{ik}(t) \quad j = i$$

where $V_{ij} \geq 0$. If $\pi_i(t)$ denotes the probability of occupying state i at time t, then the goal is to determine the asymptotic behavior of $\{x(t)\}$ as well as $\{\pi_i(t)\}$.

4. RECURRENCE ORDERS AND BALANCE EQUATIONS

In[8] we have shown that one may analyze the asymptotic behavior of such Markov chains by examining quantities which we call "recurrence orders." Let us define $\{\beta_i : i \in X\}$ by

$$\beta_i := -\infty \qquad \text{if } \sum_{t=1}^{\infty} \pi_i(t) < +\infty$$

$$:= \sup\{c \mid c \geq 0 \text{ and } \sum_{t=1}^{\infty} \varepsilon(t)^c \pi_i(t) < +\infty\} \quad \text{otherwise.}$$

If the supremum above is not attained, we will denote β_i by c^- rather than c. Let us also define

$$\beta_{ij} := -\infty \quad \text{if } \beta_i < V_{ij}$$

$$:= \beta_i - V_{ij} \quad \text{otherwise.}$$

We shall call β_i as the recurrence order of state i, and β_{ij} as the recurrence order of the transition from i to j (see[8] for more precise details).

The following fundamental result was obtained in[8].

Theorem: Balance of Recurrence Orders

For every $A \subseteq X$,

$$\sup_{i \in A, j \in A^c} \beta_{ij} = \sup_{i \in A, j \in A^c} \beta_{ji}.$$

It is worth noting that this balance equation differs fundamentally from traditional balance equations which represent balance of flow between two spatially separate sets in equilibrium. In contrast, our balance equation is for a process which is not in equilibrium; moreover it is a balance in "time."

The advantage of this balance equation is that it converts the difficult analytical problem of determining the asymptotic behavior of a time - inhomogeneous stochastic process into a purely algebraic problem of solving the balance equations.

In[9] we have obtained circulation based graph theoretic algorithms to solve these balance equations.

It has also been shown that the Markov process converges in a Cesaro-sense to the set of states with the largest recurrence orders; see[9]. Thus, the solution of the algebraic problem gives the asymptotic behavior.

It should be noted that Tsitsiklis[10] has also investigated such general Markov chains. His approach which essentially obtains bounds on the state occupation probabilities for time-invariant Markov chains, and then employs them for time-inhomogeneous chains sampled over long time intervals, is quite different from ours.

5. APPLICATION TO SIMULATED ANNEALING

Simulated annealing corresponds to the special case where $V_{ij} = [W_j - W_i]^+$. For simplicity let us suppose that the neighborhood structure is symmetric, i.e., $i \in N_j$ if and only if $j \in N_i$.

Then we have obtained a considerably stronger statement of "detailed balance", see[8].

Theorem: Detailed Balance for Simulated Annealing

$$\beta_{ij} = \beta_{ji} \quad \text{for all } j, i.$$

Using this result we have obtained in[8] the necessary and sufficient condition on the cooling rate of $\{\varepsilon(t)\}$ for simulated annealing to hit the global minimum with probability one starting from all states. It is necessary to introduce the notion of "depth" of an optimization problem.

Definition: Depth of an optimization problem

Let d be the smallest number such that for every $i \in X$, there exists a path $i = i_0, i_1, \ldots, i_{n(i)}$, with $i_{n(i)}$ a global minimizer of W, satisfying $i_{k+1} \in N_{i_k}$ for $k = 0, 1, \ldots, n(i)-1$, and such that $W(i_k) - W(i) \leq d$ for $k = 0, 1, \ldots, n(i)-1$.

Essentially, the depth measures the deepness of local minima.

In[8] we have proved the following Theorem.

Theorem: Necessary and Sufficient Conditions to Hit a Global Minimum

$$P\left\{ x(t)) \text{ hits a global minimum for some } t \geq 0 \right\} = 1$$

$$\text{if and only if } \sum_{t=1}^{\infty} \varepsilon(t)^d = +\infty.$$

Earlier, it has been shown in[11] that a similar condition is necessary for the simulated annealing Markov chain to converge in probability to the set of global minmizers. Our proof of necessity of this condition to guarantee ever hitting the global minimum is a stronger sample path statement.

In[9] we have also generalized this result to Markov chains which do not satisfy a symmetry condition, but satisfy instead what is called in[11] a "weak reversibility condition."

6. CONCLUDING REMARKS

At this stage we have a good understanding of the time vs. temperature asymptotics of simulated annealing. It is of considerable interest to study the asymptotic behavior of the simulated annealing algorithm as the size of problem instances grows, much as in the theory of computational complexity. The results obtained can be used to measure the complexity of the algorithm in probabilistic terms.

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This paper presents a novel upper bound for the second largest eigenvalue of a finite reversible time-homogeneous Markov chain as a function of three parameters, namely, the smallest transition probability, the underlying structure of the chain, and the skewness of the equilibrium distribution. This eigenvalue boudn enables us to bound the time constant of convergence of a reversible Markov chain to its equilibrium distribution. Simulated Annealing (SA), is an example of a probabilistic algorithm that is widely used for solving combinatorial optimization problems, wherein the transition probabilities are controlled by a certain temperature parameter T>0. The behavior of SA at a fixed temperature T>0 can be modeled by a reversible time-homogeneous Markov chain converging to an equilibrium distribution at that temperature. As the temperature T→0, the equilibrium distributions themselves converge to the optimal distribution. Using the results of this paper, we can not only bound the time constant of convergence of SA to equilibrium at any arbitrarily small but

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A NEW EIGENVALUE BOUND FOR REVERSIBLE MARKOV CHAINS WITH APPLICATIONS TO THE TEMPERATURE-ASYMPTOTICS OF SIMULATED ANNEALING †

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ABSTRACT

This paper presents a novel upper bound for the second largest eigenvalue of a finite *reversible* time-homogeneous Markov chain as a function of three parameters, namely, the smallest transition probability, the *underlying structure* of the chain, and the *skewness* of the equilibrium distribution. This eigenvalue bound enables us to bound the *time constant of convergence* of a reversible Markov chain to its equilibrium distribution. Simulated Annealing (SA), is an example of a probabilistic algorithm that is widely used for solving combinatorial optimization problems, wherein the transition probabilities are controlled by a certain *temperature* parameter $T>0$. The behavior of SA at a *fixed temperature* $T>0$ can be modeled by a reversible time-homogeneous Markov chain converging to an equilibrium distribution at that temperature. As the temperature $T\rightarrow 0$, the equlibrium distributions themselves converge to the optimal distribution. Using the results of this paper, we can not only bound the time constant of convergence of SA to equilibrium at any arbitrarily small but fixed temperature $T>0$, but also study the growth of this bound as $T\rightarrow 0$; thereby, providing a fairly good understanding of the *temperature asymptotics* of the simulated annealing algorithm. The eigenvalue bound of this paper is compared with the bound derived by Jerrum and Sinclair in [4]. We exhibit a class of Markov chains on which our bound, treated as a function of skewness alone, is asymptotically tighter than the Jerrum and Sinclair bound. We also show that our bound is, in general, much easier to compute for SA chains.

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1. INTRODUCTION

Let $\Omega = \{1,2, \ldots, N\}$ be a discrete *state space*, and consider a *time-homogeneous* Markov chain ($X(k)$) on Ω with an $N \times N$ probability *transition matrix* $P = [p_{ij}]$ such that for any $i, j \in \Omega$, and time $k \geq 0$,

$$p_{ij} = Prob\ (\ X(k+1)=j\ |\ X(k)=i\ ) \tag{1.1}$$

Let $v(k) = [v_i(k)]$ be the $1 \times N$ *distribution vector* describing the chain at time k such that $v_i(k) = Prob\,(X(k)=i)$; it follows that $v(k+1) = v(k)\,P$.

Suppose the Markov chain converges to an *equilibrium distribution vector* π, i.e.,

$$\lim_{k \to \infty} v(k) = \pi = \pi\,P. \tag{1.2}$$

In this paper, we are primarily interested in the speed of convergence of $v(k)$ to π. Let $1=\lambda_1 \geq |\lambda_2| \geq \cdots \geq |\lambda_N|$ denote the eigenvalues of P arranged in descending order of magnitude. It is then well known [1] that the error at time k can be bounded by

$$||v(k) - \pi|| \ \leq\ A_N\ |\lambda_2|^k \tag{1.3}$$

where $||\cdot||$ is any l_p norm and A_N is a constant independent of time k. For our purposes it suffices to consider only the l_1 norm. One can rewrite (1.3) in the form $||v(k) - \pi|| \ \leq\ A_N\ e^{-k/\tau}$ where

$$\tau \ =\ -(\log|\lambda_2|)^{-1} \tag{1.4}$$

is said to be the *time constant of convergence* of the Markov chain to its equilibrium distribution. It follows that if $|\lambda_2| \leq 1-1/q$ for some $q \gg 1$, then $\tau \leq q$. Furthermore, given any $0<\delta<1$ we will have $||v(k) - \pi|| \leq \delta$ whenever $k > [\ \log(A_N) + \log(1/\delta)\ ]\ \tau$. Therefore, the rate at which the Markov chain achieves equilibrium is determined by the time constant τ and hence by the eigenvalue of second largest magnitude λ_2.

The main result of this paper is the derivation of an upper bound on the eigenvalue of second largest magnitude of a *reversible* Markov chain. In his remarkable paper [3], Alon established the relationship between the second smallest eigenvalue $\mu_2(Q)$ of the *Laplacian matrix* Q of a graph G, and a certain *expansion parameter* $c(G)$ of the graph. A direct application of his ideas to Markov chains leads to a useful bound only for the case of *symmetric* Markov chains as shown in [2]. A symmetric Markov chain, however, can only have the *uniform* equilibrium distribution, namely, $\pi_i=1/N$ for all $i \in \Omega$. In this paper we seek a useful bound for *reversible* Markov chains which, in general, could have *non-uniform* equilibrium distributions.

The bound derived in this paper is of the form $|\lambda_2| \leq 1-1/q$, where q is related to the minimum non-zero off-diagonal entry in P, the *skewness* of its equilibrium distribution vector (a measure of the non-uniformity of the distribution defined by (2.1) in Section 2), and $\mu_2(Q)$. Recently, Jerrum and Sinclair [4] have derived an alternate bound of the form $|\lambda_2| \leq 1-\phi^2/2$, where ϕ is a certain *conductance parameter* associated with the reversible Markov chain which is an extension of the expansion idea for edge-weighted graphs. We compare the two bounds and exhibit a class of Markov chains for which our bound, treated as a function of skewness alone, is asymptotically tighter than the Jerrum and Sinclair bound.

Reversible Markov chains are of interest because they can be used to model stochastic algorithms for combinatorial optimization such as Simulated Annealing (SA) [6]. As an application of our results, we will consider using SA at a fixed temperature to solve some specific combinatorial optimization problems and derive bounds on the time constant of convergence of such chains.

The rest of this paper is organized as follows. In Section 2, we establish some notation and definitions, and present some basic results from Linear Algebra and Non-negative matrices that are required for the rest of the paper. A new upper bound for the second largest eigenvalue of a reversible

transition matrix is presented in Section 3. The SA algorithm is briefly described in Section 4 followed by a discussion of the temperature asymptotics of the corresponding reversible Markov chains. A comparison between our new bound and that derived by Jerrum and Sinclair is also made along with an analysis of the time constant of convergence of such chains. Finally, in Section 5, we summarize our conclusions.

2. PRELIMINARIES AND DEFINITIONS

We study a time-homogeneous Markov chain ($X(k)$) on a finite state space $\Omega=\{1,2,\ldots,N\}$ with transition matrix $P = [p_{ij}]$. We begin by reviewing some basic material on nonnegative matrices in general. In this paper we are using the standard graph-theoretic terminology from [5].

Definition 2.1 : The *underlying directed graph* of P is a directed graph $G_d(V, E_d)$ with vertex set $V=\Omega$, and an arc (i,j) directed from vertex i to vertex j if and only if $p_{ij}\neq 0$. The matrix P is *irreducible* if there exists a directed path from each vertex to every other vertex in its underlying directed graph G_d. For an irreducible matrix, let r denote the greatest common divisor of the lengths of all the directed cycles in its underlying directed graph. If $r=1$ the matrix is said to be *primitive*.

A primitive matrix P also has the property that there exists an integer $m>0$ such that P^m has all strictly positive entries. The Markov chain itself is said to be *irreducible (primitive)* if its transition matrix P is irreducible (primitive). Some authors refer to irreducible Markov chains as ergodic chains, and to primitive chains as regular chains. We summarize some basic facts in the following theorem from the Perron-Frobenius theory of nonnegative matrices.

Theorem 2.2 : [1] Consider an irreducible Markov chain with transition matrix P and distribution vector $v(k)$. Then

(1) $\lambda=1$ is the largest eigenvalue of P. Moreover, 1 is a simple eigenvalue.

(2) Let π be the *left* eigenvector corresponding to the eigenvalue 1 of P, i.e., $\pi = \pi P$, satisfying $\sum_{i=1}^{N}\pi_i=1$. Then $\pi_i > 0$ for all $i\in\Omega$. Furthermore, any *right* eigenvector x corresponding to any other eigenvalue $\lambda<1$ of P must be *orthogonal* to π, i.e., $\sum_{i=1}^{N}\pi_i x_i = 0$.

(3) Let γ be the *right* eigenvector corresponding to the eigenvalue 1 of P, i.e., $\gamma = P\gamma$, satisfying $\sum_{i=1}^{N}\gamma_i=1$. Then $\gamma_i = 1/N$ for all $i \in \Omega$. Furthermore, a left eigenvector corresponding to any other eigenvalue of P must be orthogonal to γ.

(4) Given any starting distribution vector $v(0)$, the distribution vector $v(k)$ at time k *converges in Cesaro sense* to π defined in (2) as $k \to \infty$, i.e., $\lim_{k\to\infty} \frac{1}{k}\sum_{l=0}^{k-1} v(l) = \pi$. If, however, the Markov chain is primitive, then $v(k)$ actually *converges* to π in the regular sense, i.e., $\lim_{k\to\infty} v(k) = \pi$.

The left eigenvector π defined in (2) above is called the *equilibrium distribution vector* of the irreducible Markov chain. It must be noted that from (4) above convergence to the equilibrium vector is guaranteed only for primitive chains. For general irreducible chains, convergence occurs only in a weak Cesaro sense.

Definition 2.3 : Consider a Markov chain with a *structurally-symmetric* transition matrix P, i.e., $p_{ij}>0$ if and only if $p_{ji}>0$. Its *underlying undirected graph* is a simple undirected graph $G(V, E)$ obtained from the underlying directed graph $G_d(V, E_d)$ by deleting all self-loops and replacing directed 2-cycles by simple edges. Thus, arcs (i,j) and (j,i) in G_d are replaced by a single edge $\{i,j\}$ in G.

Definition 2.4 : For an irreducible Markov chain with equilibrium distribution π, we define the *skewness* s_π of the chain to be

$$s_\pi = \max_{i,j\in\Omega} \frac{\pi_i}{\pi_j} \tag{2.1}$$

Clearly, s_π for an irreducible Markov chain is well defined since such a chain has $\pi_i>0$ for each $i \in \Omega$ from part (2) of Theorem 2.2. The main result of this paper deals with reversible Markov chains,

which we now define as follows.

Definition 2.5 : An irreducible Markov chain with transition matrix P and equilibrium distribution vector π is said to be *reversible* if, for all $i,j \in \Omega$, we have

$$p_{ij}\ \pi_i\ =\ p_{ji}\ \pi_j \tag{2.2}$$

A reversible Markov chain has the following interesting property. The proof is an easy consequence of the discussion above, and is therefore omitted.

Proposition 2.6 : Consider a reversible Markov chain with transition matrix P and equilibrium distribution vector π. Define $d_i = \sqrt{\pi_i}$ for each $i \in \Omega$, and the diagonal matrix $D = diag[\ d_1, d_2, \cdots, d_N\ ]$. Then,

(i) $D^2 P$ is a symmetric matrix.

(ii) $D\ P\ D^{-1}$ is a symmetric matrix.

(iii) Consequently, P is diagonalizable and has real eigenvalues.

In general, for any $K \times K$ matrix M with real eigenvalues, let $\lambda_1(M) \geq \lambda_2(M) \geq \cdots \geq \lambda_K(M)$ denote the eigenvalues of M arranged in descending order. Thus, $\lambda_1(M)$ denotes the largest eigenvalue, $\lambda_2(M)$ denotes the second largest eigenvalue etc. Using this notation, Theorem 2.2, and the above proposition, it is clear that for a transition matrix P of a reversible Markov chain we have

$$1 = \lambda_1(P) > \lambda_2(P) \geq \lambda_3(P) \geq \cdots \geq \lambda_N(P). \tag{2.3}$$

There are several symmetric matrices associated with undirected graphs. For this paper it suffices to consider only one of them.

Definition 2.7 : Given a simple undirected graph $G(V,E)$ on N vertices (i.e., no self loops and no

multiple edges). Let $deg(i)$ denote the *degree* of vertex $i \in V$ which is the total number of edges in E incident on the vertex i. Then the *Laplacian matrix* $Q(G)$ is an $N \times N$ matrix with entries defined as

$$q_{ij} = \begin{cases} deg(i) \text{ if } j=i \\ -1 \text{ if } \{i,j\} \in E. \\ 0 \text{ otherwise} \end{cases} \tag{2.4}$$

Clearly, the Laplacian matrix $Q(G)$ is a symmetric matrix. The following theorem (stated without proof) provides some more information about $Q(G)$.

Theorem 2.8 : If $G(V,E)$ is a connected simple graph with a Laplacian matrix Q, then

(1) $Q\underline{1} = \underline{0}$, where $\underline{1}$ is a vector with each entry = 1. Hence, Q has an eigenvalue 0 with eigenvector $\underline{1}$. Moreover, 0 is a simple eigenvalue of Q, i.e., $rank(Q) = N-1$.

(2) The quadratic form $x^T Q x = \sum_{\{i,j\} \in E} (x_i - x_j)^2$

(3) There exists a $N-1 \times N$ matrix B of full rank such that $Q = B^T B$.

In general, for any $K \times K$ matrix M with real eigenvalues let $\mu_1(M) \leq \mu_2(M) \leq \cdots \leq \mu_K(M)$ denote the eigenvalues of M arranged in ascending order. Thus, $\mu_1(M)$ denotes the smallest eigenvalue, $\mu_2(M)$ denotes the second smallest eigenvalue etc. From Theorem 2.8, we have Q is *positive semi-definite*, and has eigenvalues

$$0 = \mu_1(Q) < \mu_2(Q) \leq \cdots \leq \mu_N(Q). \tag{2.5}$$

The following results will prove useful in deriving our eigenvalue bound in the next section.

Lemma 2.9 (Min-max principle [13]) : If A and B are any two symmetric $K \times K$ matrices such that $A-B$ is positive semi-definite, then for each $i = 1,2,\ldots,K$, we have $\mu_i(B) \leq \mu_i(A)$.

Lemma 2.10 : Let B be any $N-1\times N$ matrix of full rank. Then, for each $i = 1,2, \ldots, N-1$, we have $\mu_i(BB^T) = \mu_{i+1}(B^TB)$.

Consequently, the smallest eigenvalue of BB^T is the second smallest eigenvalue of B^TB, the second smallest eigenvalue of BB^T is the third smallest eigenvalue of B^TB, and so on. We use these to prove the next result.

Theorem 2.11 : Let Q be any $N\times N$ symmetric and positive semi-definite matrix with $rank(Q) = N-1$, Σ be a $N\times N$ diagonal matrix with strictly positive diagonal entries, and $\sigma_{min}>0$ denote the smallest diagonal entry in Σ. Then,

(1) The $N\times N$ matrix $\Sigma Q\Sigma$ is symmetric and positive semi-definite.

(2) Also, $\mu_2(\Sigma Q\Sigma) \geq \sigma_{min}^2\mu_2(Q)$.

Proof : The proof of (1) is obvious. To prove (2), use Equation (2.4) to write $Q = B^TB$, where B is an $N-1\times N$ matrix of full rank. Define $C = B\Sigma$. Clearly C is also of full rank since Σ is a diagonal matrix with strictly positive diagonal entries. Also, $\Sigma Q\Sigma = \Sigma B^TB\Sigma = C^TC$. Therefore, by Lemma 2.10,

$$\mu_2(\Sigma Q\Sigma) = \mu_2(C^TC) = \mu_1(CC^T) \tag{2.6}$$

But $CC^T = B\Sigma^2B^T$. Also, for any vector $x\in\mathbf{R}^{N-1}$, the quadratic form

$$x^T(CC^T - \sigma_{min}^2BB^T)x = \sum_{i=1}^{N-1}(\sigma_{ii}^2-\sigma_{min}^2)y_i^2 \geq 0. \tag{2.7}$$

where we have defined $y = B^Tx$. Therefore the matrix $CC^T - \sigma_{min}^2BB^T$ is positive semi-definite by definition; hence, by Lemma 2.9, we conclude that

$$\mu_1(CC^T)\geq\sigma_{min}^2\mu_1(BB^T) \tag{2.8}$$

Applying Lemma 2.10 once again, we get

$$\mu_1(BB^T) = \mu_2(B^TB) = \mu_2(Q) \tag{2.9}$$

Combining (2.6), (2.8), and (2.9) proves this theorem.

3. A NEW EIGENVALUE BOUND FOR REVERSIBLE MARKOV CHAINS

A reversible Markov chain has a structurally-symmetric transition matrix P, and hence has an underlying undirected graph G which is both connected and simple. Furthermore, Proposition 2.6 says that P has the second largest eigenvalue $\lambda_2<1$. The main result of this paper is to obtain a tighter upper bound for λ_2 of P. This bound will be expressed in terms of the following quantities:

(1) $\alpha = \min\{ p_{ij} : i \neq j , p_{ij}>0 \}$, the smallest non-zero off-diagonal entry in P,

(2) s_π = the skewness of the equilibrium distribution π of P, and

(3) $\mu_2(Q)$ = the second smallest eigenvalue of the Laplacian matrix Q of the underlying undirected graph $G(V,E)$ of P.

Theorem 3.1 : Let $\Omega = \{1,2,\cdots,N\}$, and consider a reversible Markov chain on the state space Ω with transition matrix P, and equilibrium distribution π. Also, let α, s_π, and $\mu_2(Q)$ be as defined above. If $\lambda < 1$ is any eigenvalue of P, then

$$\lambda \leq 1 - \frac{\alpha\, \mu_2(Q)}{s_\pi} \tag{3.1}$$

Proof : Let $d_i = \sqrt{\pi_i}$ for each $i \in \Omega$, and define the $N \times N$ diagonal matrix $D = diag\ [\, d_1, d_2, \cdots, d_N \,]$. Since P is irreducible, $\pi_i > 0$ for each $i \in \Omega$ from part (2) of Theorem 2.2. Therefore $d_i>0$, D is invertible, and $D^{-1} = diag\ [\, d_1^{-1}, \cdots, d_N^{-1} \,]$.

Let $\lambda < 1$ be any eigenvalue of P and let $x \in \mathbf{R}^N$ be the corresponding right eigenvector, i.e., $Px = \lambda x$. Therefore, $x^T D^2 (I-P)x = (1-\lambda) x^T D^2 x$, which can be written as

$$1-\lambda = \frac{x^T (D^2 - W) x}{x^T D^2 x} \tag{3.2}$$

where we have defined the matrix $W = D^2 P$, i.e.,

$$w_{ij} = d_i^2 p_{ij} = \pi_i p_{ij} \tag{3.3}$$

The reversibility condition of (2.2) implies that W is symmetric. Also, the irreducibility of P implies that $W\underline{1} = D^2P\underline{1} = D^2\underline{1}$, by Theorem 2.2 part (1). Therefore, for each $i = 1,2, \ldots, N$ we have

$$\pi_i = \sum_{j=1}^{N} w_{ij} \tag{3.4}$$

Now, consider the quadratic form in the numerator of (3.2) which can be written as

$$x^T(D^2 - W)x = \sum_{i=1}^{N} (\pi_i - w_{ii})x_i^2 - \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j\neq i}}^{N} w_{ij}\, x_i\, x_j \tag{3.5}$$

Using (3.4) we get

$$x^T(D^2 - W)x = \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j\neq i}}^{N} w_{ij}\, (x_i^2 - x_i x_j) \tag{3.6}$$

Now consider $G(V, E)$ the underlying undirected graph of P. This is also the underlying graph of W, since for $j \neq i$, we have $p_{ij} \neq 0$ if and only if $w_{ij} \neq 0$. Also, $w_{ij} = w_{ji}$ since W is symmetric. Hence, (3.6) can be written as

$$x^T(D^2 - W)x = \sum_{\{i,j\}\in E} w_{ij}\, (x_i - x_j)^2 \geq \beta \sum_{\{i,j\}\in E} (x_i - x_j)^2. \tag{3.7}$$

where

$$\beta = \min \{\, w_{ij} : \{i,j\} \in E \,\}. \tag{3.8}$$

denotes the smallest non-zero off-diagonal entry in W. Define $\pi_{\max} = \max_{i\in\Omega} \pi_i$, $\pi_{\min} = \min_{i\in\Omega} \pi_i$, and

$$\alpha = \min \{\, p_{ij} : \{i,j\} \in E \,\}. \tag{3.9}$$

as the smallest non-zero off-diagonal entry in P. Since, by definition, $w_{ij} = \pi_i p_{ij}$, we immediately get

$$\beta \geq \alpha\, \pi_{\min} \tag{3.10}$$

Applying Theorem 2.8 part (2) to the right hand side of (3.7) and using (3.10) we get

$$x^T(D^2 - W)x \geq \alpha\, \pi_{\min}\, x^T Q x \tag{3.11}$$

where Q is the Laplacian matrix associated with the underlying graph G. Combining (3.2) and (3.11)

results in

$$1-\lambda \geq \alpha \pi_{\min} \frac{x^T Q x}{x^T D^2 x}. \tag{3.12}$$

It must be noted that x is a right eigenvector of P with eigenvalue $\lambda<1$, while $\pi = \underline{1}^T D^2$ is a left eigenvector of P with eigenvalue 1. Theorem 2.2 part (2) immediately shows that x and π must be orthogonal, i.e., $\underline{1}^T D^2 x = 0$. So consider the following constrained optimization problem :

Minimize $z^T Q z$ over all $z \in \mathbf{R}^N$

such that $\underline{1}^T D^2 z = 0$ and $z^T D^2 z = 1$.

Setting $y = Dz$ or $z = D^{-1}y$, the problem becomes equivalent to

Minimize $y^T D^{-1} Q D^{-1} y$ over all $y \in \mathbf{R}^n$

such that $\underline{1}^T D y = 0$ *and* $y^T y = 1$.

Recall from Section 2, that Q is a symmetric positive semi-definite matrix with eigenvalues $0=\mu_1(Q)<\mu_2(Q)\leq \cdots \leq \mu_N(Q)$. Also, $\underline{1}$ is an eigenvector of Q for eigenvalue $\mu_1(Q) = 0$. Theorem 2.11 part (1) shows that $D^{-1}QD^{-1}$ is also a symmetric positive semi-definite matrix, by treating $\Sigma = D^{-1}$ Moreover, $D^{-1}QD^{-1}\, D\underline{1} = \underline{0}$, i.e., $D\underline{1}$ is an eigenvector of $D^{-1}QD^{-1}$ with eigenvalue 0. Therefore, the above optimization problem is to minimize the quadratic form $y^T D^{-1} Q D^{-1} y$ over all *normalized* vectors $y \in \mathbf{R}^N$ that are orthogonal to $D\underline{1}$, the eigenvector corresponding to the smallest eigenvalue 0 of the matrix $D^{-1}QD^{-1}$. From quadratic programming theory [14], the minimum value of the quadratic form is clearly $\mu_2(D^{-1}QD^{-1})$, the second smallest eigenvalue of $D^{-1}QD^{-1}$. Therefore,

$$\frac{x^T Q x}{x^T D^2 x} \geq \mu_2(D^{-1}QD^{-1}). \tag{3.13}$$

Applying Theorem 2.11 part (2) to the right hand side of (3.13), with $\Sigma = D^{-1}$, gives

$$\mu_2(D^{-1}QD^{-1}) \geq \frac{1}{\pi_{\max}}\mu_2(Q) \tag{3.14}$$

So finally, combining (3.12), (3.13), and (3.14), we get

$$1-\lambda \geq \alpha \frac{\pi_{\min}}{\pi_{\max}} \mu_2(Q) = \frac{\alpha \mu_2(Q)}{s_\pi} \tag{3.32}$$

thus proving the theorem. □

For some graphs G, the second smallest eigenvalue $\mu_2(Q(G))$ is easy to compute analytically. Two examples are given below.

Cycle graphs: If G is a simple-cycle on N vertices, then the eigenvalues of its Laplacian matrix Q can be shown to be [10]

$$\mu_i(Q) = 2(1 - \cos(2\pi(i-1)/N)) \tag{3.15}$$

for each $i = 1,2, \cdots ,N$. Consequently, $\mu_2(Q) = 2(1 - \cos(2\pi/N))$ which approaches 0 as $N \to \infty$.

Hypercube graphs: If G is an n-dimensional hypercube having $N = 2^n$ vertices, then its Laplacian matrix Q has $n+1$ distinct eigenvalues [11] given by

$$\xi_m = 2m \quad ; m = 0,1,2, \ldots ,n \tag{3.16}$$

with eigenvalue $2m$ having an algebraic multiplicity $\binom{n}{m}$. Consequently, the second smallest eigenvalue $\mu_2(Q) = 2$ which is independent of N, the size of the matrix.

For graphs G in which $\mu_2(Q(G))$ is not easy to compute, one can use a lower bound derived by Alon [3] given below. This bound requires a certain expansion parameter of the undirected graph G which we now define as follows.

Definition 3.2 : Let $G(V, E)$ be an undirected graph. If $S \subset V$ is any subset of vertices in G, we

define the *deleted neighborhood* $Nbd(S)$ to be the set of vertices in $V-S$ which are joined to some vertex in S by an edge in E.

Definition 3.3 : The *expansion parameter* $c(G)$ of an undirected graph $G(V, E)$ is defined as

$$c(G) = \min \frac{|Nbd(S)|}{|S|} \tag{3.17}$$

where the minimization is performed over all subsets $S \subseteq V$ such that $0 < |S| \leq \frac{1}{2}|V|$.

Theorem 3.2 : [3] Let $G(V, E)$ be graph with Laplacian matrix Q and expansion parameter c. If $\mu > 0$ is any eigenvalue of Q, then

$$\mu \geq \frac{c^2}{4 + 2c^2} \ . \tag{3.18}$$

4. APPLICATIONS OF THE EIGENVALUE BOUND

As an application of the results of Section 3, we consider the Simulated Annealing (SA) algorithm. This algorithm was first proposed as a probabilistic algorithm for solving difficult combinatorial optimization problems [6]. It has been used with some success in problems such as VLSI layout optimization, the design of FIR filters with finite precision, and image restoration.

We describe the SA algorithm briefly. Let $\Omega = \{1, \cdots, N\}$ be a set of states with a cost function $C: \Omega \to \mathbf{R}$. The SA algorithm attempts to find a state with *globally minimum* cost. Let $x(k)$ denote the state of the algorithm at time k. With each state $i \in \Omega$, we associate a set of neighboring states $N_i \subset \Omega$, which satisfy the following assumptions:

(4.1) The neighboring sets are symmetric; that is, $j \in N_i$ if and only if $i \in N_j$.

(4.2) Given any two states i and j in Ω, there exists a finite sequence of states $i_0, i_1, \cdots, i_m$ such that $i_0 = i$, $i_m = j$, and $i_{l+1} \in N_{i_l}$, for each $l = 0, 1, \cdots, m-1$. This condition is often referred to as the *reachability* requirement.

To simply matters we make an additional assumptions which is satisfied in most applications.

(4.3) $|N_i| = \rho$ for each $i \in \Omega$, i.e., all neighbor sets are of the same size.

Suppose that the present state is $x(k) = i$. The algorithm then randomly picks a state $j \in N_i$ with probability $1/|N_i|$. If $C(j) \le C(i)$, it sets the next state to be $x(k+1) = j$. However, if $C(j) > C(i)$, it sets the next state to be $x(k+1) = j$ with probability $p = e^{(C(i)-C(j))/T}$, and $x(k+1) = i$ with probability $1-p$. In other words, if $C(j) > C(i)$, then the algorithm accepts j as the next state with probability p or remains in the present state i with probability $1-p$. The parameter $T>0$ plays the analogous role of *temperature* in the physical annnealing process. We define

$$\varepsilon = e^{-1/T} \tag{4.4}$$

to simplify notation. Note that $T = (\log\varepsilon^{-1})^{-1}$. So, if $0<T<+\infty$ then $0<\varepsilon<1$. Also, as $T\to 0$ we have $\varepsilon\to 0$.

The SA algorithm thus simulates a time-homogeneous Markov chain on state space Ω with transition matrix $P = [\, p_{ij} \,]$ with off-diagonal entries ($i\neq j$) given by

$$p_{ij} = \begin{cases} \dfrac{1}{\rho}\,\varepsilon^{[C(j)-C(i)]^+} & \text{if } j\in N_i \\ 0 & \text{if } j\in \Omega - N_i \end{cases} \tag{4.5}$$

where $[z\,]^+$ denotes the positive part of a real number z, i.e., $[z\,]^+=z$ if $z>0$, and $[z\,]^+=0$ if $z\leq 0$. The diagonal entries of P are given by

$$p_{ii} = 1 - \sum_{j\neq i} p_{ij} \tag{4.6}$$

It must be emphasized that we have assumed a *fixed temperature* $T>0$ for all time k of the SA algorithm. This is often referred to as Fixed-Temperature-Simulated-Annealing (FTSA) as opposed to a situation wherein the temperature is allowed to vary with time k according to a prespecified *cooling schedule* (see [7,8,9] for details) which results in a *time-inhomogeneous* Markov chain. In this paper, however we focus only on the FTSA algorithm.

It is easy to check that that the assumptions (4.1) and (4.2) on the neighboring sets result in P being primitive and structurally symmetric for any $0<\varepsilon<1$. Furthermore, with assumption (4.3), the equilibrium distribution vector $\pi(\varepsilon)$ can be shown (see [9]) to have entries

$$\pi_i(\varepsilon) = \frac{\varepsilon^{C(i)}}{\sum_{l=1}^{N}\varepsilon^{C(l)}} \tag{4.7}$$

which is often called the *Boltzmann distribution* at temperature $T = (\log\varepsilon^{-1})^{-1}$. Using (4.5), and (4.7), one can easily verify that the FTSA Markov chain is reversible.

Let $S^* \subset \Omega$ denote the set of all global minima. The *optimal distribution vector* π^* is a vector with entries defined as $\pi_i^* = 0$ if i is not a global minimum, and $\pi_i^* = \frac{1}{|S^*|}$ if i is a global minimum.

Temperature Asymptotics : For the FTSA chain, it is clear from (4.7) that

$$\lim_{\varepsilon \to 0} ||\pi(\varepsilon) - \pi^*|| = 0 \tag{4.8}$$

i.e., the equilibrium distribution $\pi(\varepsilon)$ approaches the optimal distribution as $\varepsilon \to 0$. For a chosen $0<\varepsilon<1$, let $\nu_\varepsilon(k)$ denote the distribution vector of the FTSA chain at time $k \geq 0$ as defined in Section 1. From Theorem 2.2 part (4) we have

$$\lim_{k \to \infty} ||\nu_\varepsilon(k) - \pi(\varepsilon)|| = 0 \tag{4.9}$$

Hence, given any arbitrary real $\delta>0$, from (4.8) and (4.9) there is an $\varepsilon>0$ and a time k_0, such that the distribution vector of FTSA (at the chosen ε) satisfies

$$||\nu_\varepsilon(k) - \pi^*|| < \delta \tag{4.10}$$

for all time $k \geq k_0$.

In this section we are primarily interested in the rate of convergence of (4.9) as a function of $\varepsilon \to 0$. We refer to this as the **temperature asymptotics** of FTSA. From the discussion in Section 1, it is clear that for a particular $\varepsilon>0$, the rate of convergence of (4.9) is governed by the time-constant of convergence τ, defined by (1.4), of the FTSA Markov chain with transition matrix P. Using (1.4) and (3.1) we now derive a bound for τ and study the behavior of this bound as $\varepsilon \to 0$.

From Theorem 3.1 we can obtain an upper bound on the eigenvalue of the transition P with second largest *algebraic* value. However, to obtain a meaningful bound on τ, the time-constant of convergence, we need an upper bound on the eigenvalue of P of second largest *magnitude*. To this end, we consider a new Markov chain corresponding to the matrix

$$\hat{P} = \tfrac{1}{2}(I+P). \tag{4.11}$$

Clearly, $\hat{P}$ has non-negative eigenvalues; thus, the algebraic value and the magnitude of an eigenvalue of $\hat{P}$ are the same. Also, $\hat{P}$ has the same equilibrium distribution as P. Furthermore, the off-diagonal entries of $\hat{P}$ are half the corresponding entries of P; hence, $\hat{P}$ is also reversible by (2.2) and has the same underlying undirected graph as P. We will therefore work with the new $\hat{P}$ instead of P.

Let us now relate the parameters used in the bound of Theorem 3.1 to the parameters of the optimization problem being solved by an FTSA Markov chain. Define

$$\Delta = \max_{i,j \in \Omega} \; | C(i) - C(j) | \tag{4.12}$$

as the maximum cost difference between any two states. Let $G(V,E)$ be the underlying undirected graph of $\hat{P}$ (or P) with Laplacian matrix Q and define

$$\delta = \max_{\{i,j\} \in E} \; | C(i) - C(j) | \tag{4.13}$$

as the maximum difference in costs between any two *neighboring* states in the Markov chain. Then, from (4.7) it follows that the skewness of the chain is given by

$$s_\pi = \varepsilon^{-\Delta} \tag{4.14}$$

The smallest non-zero off-diagonal entry of $\hat{P}$ can be computed from (4.5), (4.11), and (4.13) to be

$$\alpha = \frac{\varepsilon^{\delta}}{2\rho} \tag{4.15}$$

where ρ is the number of neighboring states for each state as given by Assumption (4.3). Using (3.1), (4.14), and (4.15) we get

$$0 \le \lambda_2(\hat{P}) \le 1 - \frac{\mu_2(Q)\, \varepsilon^{(\Delta+\delta)}}{2\rho} \tag{4.16}$$

from which one can bound the time-constant for convergence for sufficiently small ε using (1.4)

$$\tau \le \frac{2\rho}{\mu_2(Q)\, \varepsilon^{(\Delta+\delta)}} \tag{4.17}$$

as a function of ε or using (4.14)

$$\tau \leq \frac{2\rho\, s_\pi^{(1+\delta/\Delta)}}{\mu_2(Q)} \tag{4.18}$$

as a function of the skewness s_π. In case $\mu_2(Q)$ is not easily computable, one could use Alon's result of (3.42) to get

$$\tau \leq 4(1+2c^{-2})\rho\, s_\pi^{(1+\delta/\Delta)} \tag{4.19}$$

where c is the expansion parameter of the graph G. Since $\delta \leq \Delta$ by definition, one can get a less stringent bound as

$$\tau \leq 4\,(1+2c^{-2})\,\rho\, s_\pi^{\,2} \tag{4.20}$$

For a fixed optimization problem (i.e., fixed N, ρ, c, etc.), (4.20) suggests that the time-constant for convergence of the FTSA Markov chain to its equilibrium distribution with skewness s_π is $\tau = O(s_\pi^{\,2})$. In practice, usually $\delta \ll \Delta$ which yields $\tau = O(s_\pi)$. Furthermore, the bound in (3.1) may not be tight suggesting an even slower growth of τ as a function of the skewness s_π.

We now provide an example of a cost distribution on a state space for which the eigenvalue bound of (3.1) for the FTSA transition matrix is the best possible bound when treated as a function of skewness alone. We will also compare our bound with that of Jerrum and Sinclair [4] for this example. To this end we need the following definitions.

Definition 4.1 : [4] Given a reversible Markov chain on state space Ω with transition matrix P and equilibrium distribution π. The *conductance parameter* is defined as

$$\phi(P) = \min \frac{\sum_{i \in S} \sum_{j \in V-S} p_{ij}\pi_i}{\sum_{i \in S} \pi_i} \tag{4.21}$$

where the above minimization is performed over all subsets S of states with $0 < \sum_{i \in S} \pi_i \leq 1/2$.

Theorem 4.2 : [4] For a reversible transition matrix P satisfying $p_{ii} \geq 1/2$ for all $i \in \Omega$, we have

$$1 - 2\phi(P) \leq \lambda_2(P) \leq 1 - \frac{\phi(P)^2}{2} \tag{4.22}$$

Example 4.3 : Consider a simple cycle on $N=4n$ vertices as the underlying graph of a FTSA Markov chain with a cost function defined as follows :

$$C(i) = \begin{cases} i \text{ if } 1 \leq i \leq n \\ 2n+1-i \text{ if } n+1 \leq i \leq 2n \\ i-2n \text{ if } 2n+1 \leq i \leq 3n \\ 4n+1-i \text{ if } 3n+1 \leq i \leq 4n \end{cases} \tag{4.23}$$

Using these costs, $\rho = 2$, and some $\varepsilon > 0$, define the transition matrix P using (4.5) and (4.6) and set $\hat{P} = \frac{1}{2}(I+P)$. For transition matrix $\hat{P}$ it can be shown that

$$\Delta = n-1 \quad , \quad \delta = 1 \tag{4.24}$$

$$\alpha = \frac{\varepsilon}{4} \quad , \quad \textit{skewness} \quad s = \varepsilon^{-(n-1)} \tag{4.25}$$

$$\mu_2(Q) = 2(1 - \cos(\frac{\pi}{2n})) \tag{4.26}$$

$$\phi = \frac{\varepsilon^{n-1} - \varepsilon^n}{4(1 - \varepsilon^n)} \tag{4.27}$$

Thus, our bound from (3.1) gives

$$1 - \lambda_2(\hat{P}) \geq \frac{\varepsilon^n}{2} (1 - \cos(\frac{\pi}{2n})) \tag{4.28}$$

while the Jerrum and Sinclair bound from (4.22) gives

$$1 - \lambda_2(\hat{P}) \geq \frac{\varepsilon^{2n-2}}{16} \tag{4.29}$$

for sufficiently small ε and large n.

For a fixed $n>2$ (i.e., a fixed problem), it is clear that our bound in (4.28) is superior to the Jerrum and Sinclair bound in (4.29) for

$$0 < \varepsilon < \{8(1 - \cos(\pi/2n))\}^{1/(n-2)}$$

and the bound in (4.28) gets even better as $\varepsilon \to 0$. Using the lower bound in (4.22) and our bound in (4.28) and we get bounds for the time-constant for convergence to equilibrium as a function of skewness s rather than ε as

$$2s \leq \tau \leq \frac{2}{1 - \cos(\pi/2n)} s^{(1+1/(n-1))} \tag{4.30}$$

For example, if we consider $n=11$, (4.30) reduces to

$$2s \leq \tau \leq 196.5\, s^{1.1} \tag{4.31}$$

indicating that our upper bound for the time-constant τ is a fairly tight bound for large skewness s (or small ε).

The purpose of Example 4.3 was merely to illustrate an example of a reversible Markov chain for which the eigenvalue bound (hence, a bound on the rate of convergence) is fairly tight. The corresponding optimization problem, however, is very easy, since, by construction, the states 1, $2n$, $2n+1$, and $4n$ have the globally minimum cost of 1. The following example illustrates a difficult and more realistic optimization problem for which one can still use our eigenvalue bound of (3.1) to obtain a meaningful bound the time-constant of convergence of the corresponding FTSA Markov chain. Estimating the conductance parameter for this chain, however, is not straight forward; hence, the Jerrum and Sinclair eigenvalue bound of (4.22) is not directly useful in obtaining a meaningful bound for the time-constant in this case. However, with considerable ingenuity, Jerrum and Sinclair have been successful in obtaining good lower bounds for the conductance of certain classes of reversible chains [4]. Indeed, for these chains, the conductance is much larger than $O(s_\pi^{-1})$; hence, our upper-bound by

(3.1) is not tight in this case. Our bound, on the other hand is very simple to compute in general, as the following example will demonstrate, and is also tight on certain chains (as considered in Example 4.3).

Example 4.4 : Let $\{a_1 \leq a_2 \leq \cdots \leq a_n\}$ be a set of given positive integers n ascending order and define

$$K = \frac{a_1 + a_2 + \cdots + a_n}{2} \tag{4.32}$$

Let Ω denote the state space of all binary vectors of length n and consider a state $u = (u_1, u_2, \ldots, u_n)$ where $u_i \in \{0,1\}$. Define the cost of the state as

$$C(u) = \left| K - \sum_{i=1}^{n} a_i u_i \right| \tag{4.33}$$

Define the neighbors of a state u as all states differing from u in exactly one bit. Consider an FTSA algorithm to find the state of minimum cost. This is the optimization version of the SET_PARTITION problem that is known to be NP-Complete [12]. Clearly, $N = 2^n$, $\rho = n$, $\delta = a_n$, $\Delta = K$, skewness $s = \varepsilon^K$, and the underlying graph is the n-dimensional hypercube. Therefore, $\mu_2(Q) = 2$. Using (4.16) we immediately get

$$\lambda_2(\hat{P}) \leq 1 - \frac{\varepsilon^{K+a_n}}{n} \tag{4.34}$$

and from (4.18) we have a bound for the time-constant in terms of the skewness s as

$$\tau \leq n \, s^{1+a_n/K} \tag{4.35}$$

For example, if the given integers are {3,5,6,11,15}, we have $n = 5$, $a_n = 15$, and $K = 20$. From (4.35), the time-constant for an FTSA algorithm to solve the given instance to reach an equilibrium distribution of skewness $s = 10^4$ is bounded above by $\tau \leq 5 \times 10^7$ iterations.

5. CONCLUSIONS

In this paper we have derived a new upper bound on the second largest eigenvalue of a reversible Markov chain. The bound is a simple function of the skewness of the equilibrium distribution of the chain and we give examples of reversible chains where the upper bound is fairly tight. The upper bound on the eigenvalue enables us to study the time constant of convergence of the Markov chain to its equilibrium distribution. In particular, we can bound the time constant of convergence of a fixed temperature simulated annealing (FTSA) algorithm solving a particular instance of an optimization problem. Moreover, we can study the growth of this bound as the temperature approaches zero or skewness becomes arbitrarily large.

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